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BOOK OF ABSTRACTS

Photoelectromagnetic effect in lead-based perovskite crystal.....	14
Amritha A Raj <sup>1</sup> .....	14
Energy Transfer Dynamics in CsPbCl <sub>3</sub> Perovskite Doped with Various Contents of Yb <sup>3+</sup> .....	15
Lamiaa Abdelrazik .....	15
Optimization of Electron Transport Layers for p-i-n Perovskite Solar Cells.....	16
Erik Ahlswede .....	16
Sublimed Fullerene for repeatable and efficient perovskite-based solar cells .....	17
Ahmed Ahmed.....	17
Tailoring the Optoelectronic Properties of Tin-Based Perovskite Light- Emitting Diodes in Nonoxidative Solvent .....	18
Ece Aktas <sup>1</sup> .....	18
Achieving nearly 100% quantum-efficient lead-free perovskite solar cells with 34.67% power-conversion efficiencies through band and defect engineering-based material design optimization.....	19
Al Dajani Saleem <sup>1,2,3</sup> .....	19
Functional P-I-N perovskite solar cell using low-damage pulsed laser deposited tin (IV) oxide electron transport layer.....	21
Kilian Alcocer <sup>1</sup> .....	21
CsPbI <sub>2</sub> Br Intermediate Phase Effect of Final Film Quality: Crystallinity, Morphology, And Phase Purity.....	22
Esra Alhabshi .....	22
Optimization Of Wide And Narrow Bandgap Absorbers For All-Perovskite Tandem Solar Cell .....	23
Jules Allegre .....	23
Analysis of the functionalization of ITO layers with SAMs by Inverse PES to understand ...	24
Jules Allegre.....	24
Unveiling the Degradation Mechanism of Hybrid Tin-Lead Perovskites .....	25
Asayil Alsulami <sup>1</sup> .....	25
Quantifying Defects in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Perovskite Solar Cells using Capacitance Spectroscopy Techniques.....	26
Nisheka Anadkat <sup>1*</sup> .....	26
Enhanced optoelectronic coupling for monolithic perovskite/silicon tandem solar cells .....	27
Erkan Aydin <sup>1</sup> .....	27
The Effect of Antimony Substitution on the Optoelectronic Properties of MAPbI <sub>3</sub> .....	28
Folusho Helen Balogun <sup>1</sup> .....	28
An underwater city solar: high-band gap bromide-based perovskite solar cells for underwater application .....	29
Jessica Barichello <sup>1</sup> .....	29

Charge Localization in Cs <sub>2</sub> AgBiBr <sub>6</sub> Halide Double Perovskite: Small Polarons and Self-Trapped Excitons .....	30
Mehmet Baskurt* .....	30
Sequentially hybrid vacuum-processed Multi-Cation Halide Perovskite .....	31
Felix Battran <sup>1</sup> .....	31
Scalable Perovskite Top Cells for Monolithic PSTSCs .....	32
T. Bertram <sup>1*</sup> .....	32
Passivation of defects in perovskite solar cell using Enamine Analogue of Tetra-Phenylethylene: A New Systematic Pathway to Achieve High Performance .....	33
Shubhangi Bhardwai <sup>1</sup> .....	33
Scaling of Perovskite Silicon Tandem Solar Cells – Progress and Challenges.....	34
Juliane Borchert <sup>1,2</sup> .....	34
Bifacial Module for 4-Terminal Hybrid Tandem .....	35
Rosemary Bramante <sup>1,2</sup> .....	35
Unraveling the Mysteries of Potential-Induced Degradation: A Precise Method for Revealing Critical Insights on Perovskite Solar Cells .....	36
Robbe Breugelmans <sup>1,2,3</sup> .....	36
Distinguishing Carrier Transfer and Recombination at Perovskite-Transport Layer Interfaces Using Time-Resolved Spectroscopy.....	37
Edward Butler-Caddle <sup>1</sup> .....	37
How to get over 25.5mA cm <sup>-2</sup> integrated current density in perovskite solar cells and modules: substrate choice, annealing, additives and passivation strategies investigation .....	38
Luigi Angelo Castriotta <sup>1</sup> .....	38
New insights for developing lower-toxicity and stable inkjet-printable perovskite precursor inks for fully-printed annealing-free perovskite PVs manufacturing .....	39
Dimitris A. Chalkias <sup>1,2</sup> .....	39
Cesium Tin Halide based Absorber Layers for Graphene-derived all- inorganic Flexible Perovskite Solar Cells.....	40
Subhash Chander* <sup>1</sup> .....	40
NiOx nanoparticle including in hole transport layer of inverted p-i-n perovskite solar cell for improvement of its stability.....	41
Jakapan Chantana <sup>1</sup> .....	41
Organic chloride salt incorporated SnO <sub>2</sub> electron transport layers for improving the performance of perovskite solar cells.....	42
Zhigang Che .....	42
Functional Multicomponent Nanocrystal Superlattices Comprising Lead Halide Perovskite Nanocrystals .....	43
Ihor Cherniukh <sup>1,2</sup> .....	43

Defect Passivation Effects in 2-D Halide Perovskite Field-Effect Transistor by Lewis-base Molecules. ....	44
Hyeonmin Choi <sup>1</sup> .....	44
Investigation of Time and Location Dependent Variations in Electroluminescence Images of Perovskite Solar Cells .....	45
Ennio Luigi Comi <sup>1</sup> .....	45
Optimal Interface Engineering through SAM Energy Alignment and Functionalization.....	46
Hannah Contreras .....	46
Investigation of the band alignment at the interface between 2D/3D halide perovskite films and charge extraction layers.....	47
Pia Dally <sup>1</sup> .....	47
Integrated: experimental and theoretical study on structural and magnetic properties of thin films of double perovskite ruthenates; Ba <sub>2</sub> DyRuO <sub>6</sub> & Sr <sub>2</sub> DyRuO <sub>6</sub> .....	48
Sahil Dani <sup>1</sup> .....	48
Engineering polycrystalline Ruddlesden Popper perovskite to achieve wavelength dependent photodetector.....	49
Parsa Darman <sup>1</sup> .....	49
Visualizing Macroscopic Inhomogeneities in Perovskite Solar Cells .....	50
Akash Dasgupta <sup>1</sup> .....	50
Advanced study of carrier transport in lead-free double perovskite materials .....	51
Elke Debroye <sup>2</sup> .....	51
Visualizing buried interfaces in solution-processed perovskites.....	52
Marielle Deconinck <sup>1,2,3</sup> .....	52
Cation passivation and 2D/3D heterostructure: strategies toward high efficient and stable perovskite solar cells .....	53
Matteo Degani <sup>1</sup> .....	53
Suppressed Ionic Migration Effects in Mixed Lead-Tin Halide Perovskite Semiconducting Devices .....	54
Krishanu Dey <sup>1</sup> .....	54
Investigating the viability of solution processed metal oxides as the hole-extracting layer in tin perovskite photovoltaics.....	55
Matthew Dingley.....	55
Photophysics of Tin-Lead Halide Perovskites for Tandem Photovoltaics.....	56
Nicole Dong <sup>1</sup> .....	56
Structure and properties investigations of carbazole-based monolayers with different functional groups for perovskite solar cells.....	57
Aida Drevilkauskaitė .....	57
Factors Affecting Combined Thermal and Light Stability of Inverted Architecture Formamidinium-Cesium Lead Triiodide Perovskite Solar Cells .....	58

James N. Drysdale <sup>1</sup> .....	58
In-situ characterization of metal halide perovskite formation from environmentally friendly solvents using in situ wide and small angle X-ray scattering .....	59
Alan D. F. Dunbar <sup>1</sup> .....	59
Investigating the Interplay between Microstructure and Carrier Dynamics in Two-Dimensional Perovskites .....	60
Lisanne Einhaus .....	60
Interface and Device Engineering Toward High Performance Flexible Perovskite Solar Cells	61
Muhammad Fahim <sup>1*</sup> .....	61
Probing and quantifying Förster-like energy transfer from single perovskite quantum dots to organic dyes.....	62
Leon G. Feld, <sup>1,2</sup> .....	62
Electrostatically triggered autonomous self-healable and stretchable hydrogel for flexible perovskite solar cells .....	63
Irum Firdous <sup>1*</sup> .....	63
Designing Ytterbium-doped perovskite near-IR emitters: the role of dimensionality and crystal geometry .....	64
Giulia Folpini <sup>1</sup> .....	64
Transient Electroabsorption Spectroscopy Reveals Direct Tracking and Extraction of Charge Carriers from Hybrid Perovskites.....	65
Marius Franckevičius <sup>1</sup> .....	65
Using the Ionic Liquids (ILs) as the Additives to Enhance the Perovskite Solar Devices Stability and Efficiency.....	66
Xiao-Xin Gao .....	66
Experimental determination of exciton binding energy, exciton-phonon interaction and Urbach energy in $\gamma$ -CsPbI <sub>3</sub> nanoparticles.....	67
Daniel L. Gau <sup>1</sup> .....	67
Evaporation-Solution Deposition of >20% Efficient FAPbI <sub>3</sub> -Based Perovskite Solar Cell as Mid-cell for Triple Junction Solar Cells.....	68
Mohammadreza Golobostanfard.....	68
Treatment of perovskite solar cells by cesium chloride: towards inorganic Ruddlesden-Popper phase passivation for hybrid perovskite .....	69
Thomas Gomes.....	69
Interlayer engineering enhances responsivity of perovskite lateral photoconductors for X-ray detectio .....	70
Isabel Gonçalves <sup>1</sup> .....	70
Achieving Balanced Charge Extraction via Concerted Co-Doping of Charge- Selective Layers for Stable CsPbI <sub>3</sub> Solar Cells.....	71
Thomas W. Gries <sup>1,2</sup> .....	71

Learning curves from long-term outdoor testing and indoor optoelectronic characterization of perovskite mini-modules .....	72
Maria Hadjipanayi <sup>1</sup> .....	72
The effect of solution phase bromide-iodide exchange on the structural and optoelectronic properties of Cs <sub>3</sub> Cu <sub>2</sub> Br <sub>5</sub> layers .....	73
Hajdu Cintia .....	73
Interface formation between halide perovskites and NiOx studied by photoemission spectroscopy .....	74
Javid Hajhemati <sup>1,2</sup> .....	74
Expanding the Compatibility of P3HT Hole Transport Layers for Stable Perovskite Solar Cells .....	75
David Hardy <sup>1</sup> .....	75
Reversible Thermochromic Self-trapped Excitonic Emission in One Dimensional Tin-based Halide Perovskite Thin Film.....	76
Yanmei He <sup>1</sup> .....	76
Defect passivation of 2D tin perovskites for lasing applications .....	77
Yarong He <sup>1</sup> .....	77
Unraveling the Defects Passivation During Perovskite Vacuum Co-deposition by In-situ Grazing-Incidence X-ray Scattering and Photoluminescence.....	78
V. Held <sup>1</sup> .....	78
Where does the current flow? – Spatial inhomogeneity of the reverse bias current and its impact on degradation .....	79
J. Henzel <sup>1,2</sup> .....	79
Development of Perovskite Absorbers for Application in Perovskite/Perovskite/Silicon Triple-Junction Solar Cells.....	80
Minasadat Heydarian <sup>1,2</sup> .....	80
Spacer Layer Dependent AC conductivity of Two-dimensional Dion-Jacobson Halide Perovskites .....	81
Nisha Hiralal Makani <sup>1</sup> .....	81
Exploring the Energetic Landscape of Mixed Iodine-Bromide Perovskites.....	82
Yvonne J. Hofstetter <sup>1,2</sup> .....	82
Towards commercialisation with lightweight, flexible perovskite solar cells for residential photovoltaics .....	83
Philippe Holzhey <sup>1+</sup> .....	83
A novel, lead-free halide perovskite derivative for ferro- and piezo- electric applications .....	84
Esther Y.-H. Hung <sup>1</sup> .....	84
Static Moisture induced structural and optical evolution of 2D and 3D perovskites.....	85
Rohitkumar Jadhav <sup>1*</sup> .....	85
Perovskite-based bifacial and flexible tandem solar cells .....	86

Inyoung Jeong <sup>1</sup> .....	86
FAPbI <sub>3</sub> -based perovskite thin film using Co-evaporation method .....	87
Minji Jeong* .....	87
Alumina nanoparticle interfacial buffer-layer for narrow bandgap perovskite solar cells.....	88
Heon Jin <sup>1</sup> .....	88
Development of luminescent halide perovskite films through CSS.....	89
Isabella Antony Kalluvila Justin <sup>1</sup> .....	89
Dimethylammonium-incorporated mixed halide perovskite nanocrystals for stabilized red emission.....	90
Shaoni Kar <sup>1,2</sup> .....	90
Development of n-type self-assembled monolayers for performance enhancements of perovskite solar cells.....	91
Masahiro Kashiwazaki <sup>1,2</sup> .....	91
Light Makes Right: Laser Polishing for Surface Modification of Perovskite Solar Cells.....	92
Mayank Kedia <sup>1,2</sup> .....	92
Copper(I) selenocyanate: A Solution-processed Hole Transport Layer for Organic and Perovskite Solar Cells.....	93
Rashi Kedia .....	93
Plasma damage-free deposition of transparent top cathode using linear facing target sputtering for semi-transparent perovskite solar cells .....	94
Han-Ki Kim .....	94
Study on Charge Carrier Transport in HTL via Optoelectronic Analysis .....	95
Sunkyu Kim <sup>1</sup> .....	95
Modulating Electrical Conductivity of Metal Halide Perovskite Thin Films through Surface Metal Halide Deposition .....	96
Yongjin Kim <sup>1</sup> .....	96
Mode locking of hole spin coherences in CsPb(Cl,Br) <sub>3</sub> perovskite nanocrystals generated via positively charged excitons .....	97
Erik Kirstein <sup>1</sup> .....	97
Using Bayes' Theorem to Evaluate Time-Resolved Photoluminescence Data .....	98
Manuel Kober-Czerny.....	98
Atmospheric neutron resilience of flexible perovskite solar cells with thoughtfully designed organic hole transport material.....	99
Giulio Koch <sup>1</sup> .....	99
Developments for the industrialization of graphite-based, in-situ crystallized perovskite solar cells.....	100
Markus Kohlstädt <sup>1</sup> .....	100
Encompassing Tetrafluoroborate Anion into FAPbI <sub>3</sub> Photoabsorber Layer for Efficient and Stable Perovskite Solar Cells.....	101

Daisuke Kubota <sup>1,2</sup> .....	101
“Horse measurement” for accurate quantification of information on the charge dynamics in halide perovskites .....	102
Jitendra Kumar <sup>1</sup> .....	102
Coordinated Image and Bulk Electrical Characterisation for Better Elucidating the Role Heterogeneity Plays in Perovskite Solar Cell Degradation.....	103
Jamie S Laird <sup>1</sup> .....	103
Sustainable and Circular Management of Perovskite Solar Cells via Green Recycling .....	104
Valentina Larini <sup>1</sup> .....	104
Surface or Bulk Defects - Halide Perovskites Probed by Photothermal Deflection Spectroscopy .....	105
Martin Ledinsky .....	105
Strategies for low threshold and photo-stable amplified spontaneous emission from halide perovskite thin films .....	106
Gayoung Lee <sup>1</sup> .....	106
Elucidating Photostability of the Perovskite Films via Anti-Solvent Additive passivation..	107
Wonjong Lee <sup>1</sup> .....	107
Efficient all-thermally evaporated perovskite light emitting diodes for active matrix displays .....	108
Jinghui Li <sup>1</sup> .....	108
Combinatorial slot-die coating of metal halide perovskite solar cells.....	109
Jinzhao Li <sup>1,2</sup> .....	109
In-situ analysis of solvent extraction process for large area perovskite film formation .....	110
Xuan Li .....	110
Understanding the Space Charge Limited Current in Metal Halide Perovskite (SCLC).....	111
Jongchul Lim <sup>1</sup> .....	111
Efficient HTL-free Perovskite Solar Cells via Surface P-type Doping.....	112
Benyu Liu <sup>1</sup> .....	112
Exploiting the Synergies - p-i-n Carbon Perovskite Solar Cells with Fully Ambient Pressure Compatible Processes .....	113
Tino Lukas <sup>1</sup> .....	113
Two-Step Hybrid Perovskite Deposition: a Novel Crystal Engineering Approach and Vacuum-processed HTLs for Tandem Solar Cells.....	114
Erica Magliano <sup>1</sup> .....	114
Mixed Monolayers as a Strategy to Improve the Performance of the Perovskite Solar Cells	115
Artiom Magomedov <sup>1,2</sup> .....	115
Novel low-temperature laminable encapsulants based on two- dimensional hexagonal boron nitride for perovskite solar cells and modules .....	116
Paolo Mariani <sup>1</sup> .....	116



Single crystal 2D perovskite thin films for solar cells .....	118
Daniela Marongiu <sup>1</sup> .....	118
2D layered hybrid perovskites featuring benzotriazole-based organic cations: a fundamental study of structural and optical properties .....	119
Arthur Maufort <sup>1</sup> .....	119
Dipole modification of the perovskite/C60 interface upon piperazinium iodide treatment - a Near-UV photoemission spectroscopy study.....	120
Dorothee Menzel <sup>1</sup> .....	120
Origin of the Voc growth in perovskite solar cell with Br substitution.....	121
Ganghong Min <sup>1,2</sup> .....	121
Two-step evaporation of low-bandgap mixed lead-tin perovskites for solar cells .....	122
George A. Morgan .....	122
Multifunctional Leek-Inspired Light Management Layer for improving the performance of perovskite solar cells .....	123
Seyede Maryam Mousavi <sup>1</sup> .....	123
Unrevealing Defects during Lead-Halide Perovskite Film Formation.....	124
Nada Mrkyvkova <sup>1</sup> .....	124
Scalable Fabrication of Pure Formamidinium based Perovskite Solar Cells by Slot- Die Coating Process.....	125
Kunnummal Mangott Muhammed Salim <sup>1*</sup> .....	125
Defect tolerance and improved stability in 1.8 eV bandgap perovskite solar cells activated by Ionic Liquid Passivation.....	126
Artem Musiienko <sup>1</sup> .....	126
Thermal disorder-induced carrier localisation activates reverse halide segregation.....	127
Nursultan Mussakhanuly <sup>1</sup> .....	127
Unveiling the translational impact of electron transport layers on perovskite film formation.	128
Stefan Nicholson <sup>1,2</sup> .....	128
Strategy for in-air deposition of perovskite cell and modules: Comparison between TiO <sub>2</sub> and SnO <sub>2</sub> transporting layers .....	129
Hafez Nikbakht <sup>1*</sup> .....	129
N-Octylammonium Bis(trifluoromethylsulfonyl)imide as a Highly Functional Additive for Spiro-OMeTAD Layer in Perovskite Solar Cells.....	130
Naoyuki Nishimura <sup>1</sup> .....	130
CsPbI <sub>3</sub> towards Tandem application.....	131
Elisa Nonni <sup>1</sup> .....	131
Flash Annealed Nickel Oxide for Large Area Perovskite Solar Cells.....	132
Efrain Ochoa-Martinez <sup>1</sup> .....	132

Polarimetric measurements of the bright triplet emission of single cesium lead halide perovskite quantum dots at cryogenic temperature .....	133
Virginia Oddi <sup>1,2</sup> .....	133
Fundamental analysis of all inorganic germanium perovskite .....	134
Andrea Olivati <sup>1,2</sup> .....	134
Lead-free Magnetic Halide Perovskite Photovoltaics .....	135
Sanika S. Padelkar <sup>#1,2,3</sup> .....	135
Innovative concepts to improve optical gain in CsPbBr <sub>3</sub> perovskite thin films .....	136
Ulrich Paetzold .....	136
Bandgap Engineering of Two-Step Processed Perovskite Top Cells for Application in Perovskite-Based Tandem Photovoltaics.....	137
Ronja Pappenberger <sup>1</sup> .....	137
Characterization of perovskite layers using photoconductance techniques .....	138
Gábor Paráda <sup>1</sup> .....	138
Characteristics of Stable Inorganic CsPbI <sub>3</sub> Perovskite films deposited by thermal evaporation .....	139
Jihye Park <sup>1</sup> .....	139
Pulsed laser deposition of inorganic halide perovskite thin films with various compositions	140
Elsa Parrat <sup>1</sup> .....	140
Analog Memristor of Cs <sub>4</sub> CuSb <sub>2</sub> Cl <sub>12</sub> Perovskite Nanocrystals as Solid- State Electronic Synapse.....	141
Sumaiya Parveen <sup>1</sup> .....	141
Boosting device performance of low-dimensional perovskite solar cells by ionic liquid engineering .....	142
Vani Pawar <sup>1</sup> .....	142
Synthesis of CsPbBr <sub>3</sub> Nanocrystals Employing a New X-Type Ligand Based on Sulphur-atom. ....	143
Meenakshi Pegu <sup>1</sup> .....	143
Mitigating performance losses in perovskite solar cells incorporating ionic transport layers	144
W. Hashini K. Perera <sup>1</sup> .....	144
Nanoparticles for improved wettability and enhanced carrier lifetimes of perovskites on hydrophobic self-assembled monolayers .....	145
W. Hashini K. Perera <sup>1</sup> .....	145
Asymmetric triphenylethylene-based hole transporting materials for highly efficient perovskite solar cells.....	146
Julius Petrulevičius <sup>1</sup> .....	146
How Substrate Surface Passivation Dictates Preferential Growth of Thermally Co-Evaporated Perovskite Thin Films.....	147
Julian Petry <sup>1</sup> .....	147

Advanced Laser-Patterned Interconnection Concepts for Perovskite (Tandem) Solar Modules .....	148
Julian Petry .....	148
Effect of charge extraction layer on optoelectronic properties of perovskite via Photoluminescence Imaging .....	149
Himanshu Phirke <sup>1</sup> .....	149
Interface study between transport layers by atomic layer deposition and FA-based perovskites .....	150
Bhavya Rakheja <sup>1</sup> .....	150
Pronounced Room-Temperature Vibrational Coherence Coupled to Electronic Transitions in Cs <sub>2</sub> Au <sub>2</sub> Br <sub>6</sub> .....	151
Sankaran Ramesh <sup>1</sup> .....	151
The influence of the chemical composition of 3D perovskites on the formation and stability of 2D/3D structures.....	152
Murillo Henrique de Matos Rodrigues <sup>1</sup> .....	152
Monolithic Perovskite/Silicon Tandem Solar Cells Prepared by Thermal Co-Evaporation with Optimized Top Cell Band Gap .....	153
M. Roß <sup>1</sup> .....	153
Wind effects on the performance and hysteresis of building-integrated perovskite solar cells	154
Hadi Rostamzadeh <sup>1,2</sup> .....	154
Thermally Stable and Water-resistant using All-Inorganic CsPbI <sub>2</sub> Br Perovskite Solar cells	155
Rajarshi Roy* <sup>1</sup> .....	155
Unravelling Lead Free Perovskites for White Light Emission by Charge Carrier Localization Amongst the Lattice Structure.....	156
Monika Salesh .....	156
The effect of halide composition on the luminescent properties of cesium-copper halide pseudo- perovskites.....	157
Gergely F. Samu <sup>1</sup> .....	157
Tuning the electronic structure of SnO <sub>2</sub> via Mg-doping for application in perovskite solar cells .....	158
Sannino Gennaro Vincenzo <sup>1,2</sup> .....	158
The influence of surface treatments on the efficiency and stability of 1.68eV bandgap triple-halide perovskite solar cells .....	159
Florian Scheler <sup>1</sup> .....	159
Anharmonicity of the lead–halide bond in chlorine-substituted MAPbI <sub>3</sub> in comparison to MAPbBr <sub>3</sub> .....	160
Götz Schuck <sup>1</sup> .....	160
Chloride-based additive engineering for efficient and stable wide-bandgap perovskite solar cells.....	161
Xinyi Shen <sup>1</sup> .....	161

Chlorine Incorporation for Scalable 1.8 eV Wide Bandgap Perovskite Solar Modules with Enhanced Efficiency and Photostability .....	162
Severin Siegrist* .....	162
Optimising sputtering conditions to fabricate SnO <sub>2</sub> films as a reliable electron transport layer for perovskite solar cell .....	163
Abhinav Kumar Singh <sup>1</sup> .....	163
Impact of Ion Migration on the Operational Stability of Perovskite Solar Cells: Insight from Photoemission Spectroscopy .....	164
Shivam Singh <sup>1,2</sup> .....	164
Mitigating phase segregation in co-evaporated wide band gap perovskite films for perovskite-silicon tandem application .....	165
Viktor Škorjanc <sup>1</sup> .....	165
The Impact of Surface Termination of MAPbI <sub>3</sub> Perovskite on the Electronic Structure at Interface with Rubrene .....	166
Nicholas Sloane <sup>1</sup> .....	166
Two-step MAPbI <sub>3</sub> deposition by low-vacuum proximity-space-effusion for high-efficiency inverted semitransparent perovskite solar cells .....	167
Emanuele Smecca <sup>1</sup> .....	167
Characterising halide perovskite crystallisation using in situ GIWAXS .....	168
Joel A. Smith <sup>1</sup> .....	168
The problem of vanishing photocurrent in inorganic, wide band gap CsPbBr <sub>3</sub> perovskite solar cells .....	169
Zbigniew Starowicz <sup>1</sup> .....	169
Industrially Compatible FAPI Perovskite Solar Cells and Modules Fabrication by Meniscus Coating Technique .....	170
Maurizio Stefanelli <sup>1*</sup> .....	170
Superacid treatment of metal halide perovskites to improve the absorber/hole transport layer interface .....	171
Thomas Stergiopoulos <sup>1</sup> .....	171
Multi-Stage Phase-Segregation of Mixed Halide Perovskites under Illumination: A Quantitative Comparison of Experimental Observations and Thermodynamic Models .....	172
K. Suchan <sup>1</sup> .....	172
Surface treatment for efficient and durable formamidinium lead iodide (FAPbI <sub>3</sub> ) perovskite solar cells .....	173
Jiajia Suo <sup>1,2*</sup> .....	173
Interpreting Halide Perovskite Semiconductor Photoluminescence Kinetics .....	174
Margherita Taddei .....	174
3D/2D heterojunction for efficient and stable perovskite solar cells based on chemical bath deposition SnO <sub>2</sub> electron transport layers .....	175
Shun Tian <sup>1</sup> .....	175

Encapsulation and Stability of Emerging Photovoltaic Technologies Outdoors in the UK...	176
Bening Tirta Muhammad*	176
Vacancy Ordered Double Perovskite Caged 2D- Light Absorbing Perovskite for Optical Humidity Sensing	177
Abinash Tiwari	177
2d/3d Perovskite Heterojunction Solar Cells: Pairing Performance With Stability	178
Francesco Toniolo <sup>1</sup>	178
Driving Lattice Dynamics in 2D Perovskites via THz Kerr Effect	179
Joanna M. Urban <sup>1</sup>	179
Synergistic approach towards enhanced stability and emission of FAPbBr <sub>3</sub> NCs for LED applications	180
Liam Van Gaal <sup>1</sup>	180
Tailoring Interlayer Charge Transfer Dynamics in 2D Perovskites with electroactive ligands	181
Wouter Van Gompel <sup>1</sup>	181
Light dependency for current - voltage curve hysteresis in perovskite solar cells modelled by slow - shallow trap states	182
W. Veurman	182
Stabilizing Perovskite Solar Cells via Compressive Strain	183
Hao Wang <sup>1</sup>	183
Mastering the crystallization dynamic of FAPbI <sub>3</sub> thin film for high efficiency and stable light-emitting diodes	184
Dr. Heyong Wang <sup>1</sup>	184
Device Physics of Ion-defect-coupled Perovskite LEDs	185
Yu Wang <sup>1</sup>	185
Vacancy-mediated Cs <sup>+</sup> and Br <sup>-</sup> ion migration in biaxially strained CsPbBr <sub>3</sub>	186
Matthew J. Wolf <sup>2</sup>	186
The influences of excess FAI to ASE performances and carrier dynamics in FAPbI <sub>3</sub> perovskite	187
Chun-Sheng Wu <sup>1,2</sup>	187
Carrier-Phonon Interaction Induced Negative Thermal-Optic Coefficient at Near Band Edge of Quasi-2D (PEA) <sub>2</sub> PbBr <sub>4</sub> Perovskite	188
Sheng-Chan Wu <sup>1,2,3</sup>	188
Lead-Absorbing ionogel-based encapsulation for impact-resistant, stable, and lead-safe perovskite modules	189
Xun Xiao	189
Dally	190
Enhanced Hole Injection via Perovskite Band Alignment for High- Performance Blue light-emitting diode	190
Yuting Xu <sup>1,2</sup>	190

Thermal Stability of Perovskite Solar Cells with Ionic liquid dopant to Spiro-OMeTAD ...	191
Kohei Yamamoto .....	191
Perovskite orientation growth and bandgap optimization via thermal evaporation.....	192
Jin Yan <sup>1,2</sup> .....	192
A Templating Approach to Controlling the Growth of Co-evaporated Halide Perovskites...	193
SiYu Yan .....	193
Manipulation of the optoelectronic properties of layered hybrid perovskites by molecular intercalation.....	194
Linjie Yang <sup>1</sup> .....	194
Laminated Perovskite Solar Cells with Enhanced Stability and Performance via Thermocompression Bonding .....	195
Tae-Youl Yang <sup>1</sup> .....	195
Impact of charge transport at the interfaces of lead halide perovskite solar cells .....	196
Sarah Su-O Youn <sup>1</sup> .....	196
Thermally Stable All-vacuum-deposited Perovskite Solar Cells with Copper Phthalocyanine Hole Transport Layer .....	197
Qimu Yuan <sup>1</sup> .....	197
Enhanced Hole Mobility of p-Type Materials by Molecular Engineering for Efficient Perovskite Solar Cells .....	198
Ceylan Zafer <sup>1*</sup> .....	198
Study of co-evaporated $\alpha$ -FAPbI <sub>3</sub> perovskite growth as function of time and temperature deposition .....	199
Francesca Zarotti <sup>1</sup> .....	199
Manipulation of Crystal Orientation and Phase Distribution of 2D Perovskite through Synergistic Effect of Additive Doping and Spacer Engineering .....	200
Xiao Zhang <sup>1</sup> .....	200
Ultrathin semitransparent perovskite solar cells .....	201
Zongbao Zhang <sup>1,2</sup> .....	201
A robotic platform assisted perovskite materials synthesis.....	202
Haitao Zhao .....	202
Many-body Correlations and Exciton Complexes in CsPbBr <sub>3</sub> Quantum Dots .....	203
Cheglan Zhu <sup>1,2‡</sup> .....	203
Impact of Low-Temperature Seed-Assisted Growth on the Structural and Optoelectronic Properties of MAPbBr <sub>3</sub> Single Crystals .....	204
Waqas Zia <sup>1,2</sup> .....	204
Optical and electrical optimization of the electron-selective top contact for perovskite single-junction and perovskite/silicon tandem solar cells.....	205
Lea Zimmermann <sup>1</sup> .....	205

# Photoelectromagnetic effect in lead-based perovskite crystal

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The Lead-based MAPbI<sub>3</sub> single crystals are reported to have low trap densities and long carrier diffusion lengths [1] due to which they possess remarkable photovoltaic quality comparable to silicon. Two major semiconductor properties that quantify the efficiency are the bulk lifetime (depends on the recombination of electrons and holes in the crystal, accounting for the material quality) and surface recombination velocity (depends on the interface between the materials and their boundaries, accounting for the fabrication process) [2]. In our research, the photoconductance and the short circuit photoelectromagnetic current are used to obtain the excess carrier bulk lifetime and the surface recombination velocity in MAPbI<sub>3</sub> single crystal.

The PEM effect is one of the oldest known techniques for estimating carrier properties in semiconductors [4]. When light falls on a semiconductor surface, photo-diffused electrons and holes get deflected in opposite directions in the presence of a perpendicular magnetic field inside the semiconductor. This generates a PEM voltage (figure 1a). This is dependent on the applied magnetic field, the photon flux ( $I_0$ ), and the diffusion length ( $\mu L$ ) (fig 1(b) and (c)).

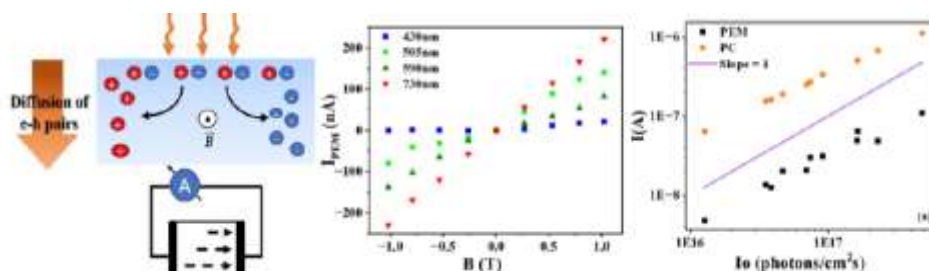


Figure 1 (a) PEM phenomenon (b) Magnetic dependence of PEM (c)  $I_0$  dependence of PEM and PC

The photocurrent is proportional to the mobility-lifetime ( $\mu\tau$ ) product, and the PEM short circuit current is proportional to the product of the mobility times the carrier diffusion length ( $\mu L$ ). When one takes the ratio of both, one can yield the bulk carrier lifetime independent of the light intensity (due to similar  $I_0$  dependence as shown in the log-log plot in figure (1 (c)) and surface recombination velocity.

We could estimate the bulk lifetime ( $6\mu s$ ), carrier diffusion length ( $32\ \mu m$ ) and SRV ( $1000\text{cm/s}$ ) for the single crystal. [3]

[1] Q. Dong et al., *Science* (1979), vol. 347, no. 6225, pp. 967–970, Feb. 2015, doi:10.1126/science.aaa5760.

[2] M. De Laurentis and A. Irace, *Journal of Solid State Physics*, vol. 2014, no. 11m, pp. 1–19, 2014, doi:10.1155/2014/291469.

[3] S. W. Kurnick and R. N. Zitter, *J Appl Phys*, vol. 27, no. 3, pp. 278–285, 1956, doi:10.1063/1.1722357.

[4] T. S. Moss, *Semiconducteurs et Phosphores*, 1958, pp. 98–112. doi: 10.1007/978-3-663-02557-3\_7.

# Energy Transfer Dynamics in CsPbCl<sub>3</sub> Perovskite Doped with Various Contents of Yb<sup>3+</sup>

Lamiaa Abdelrazik

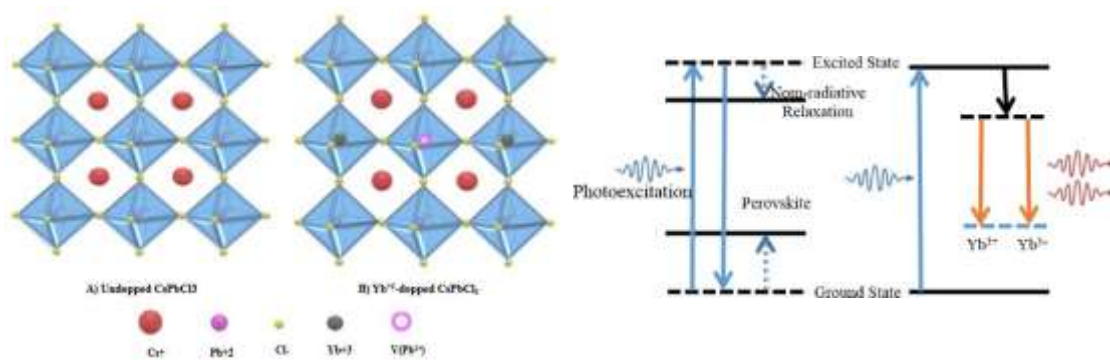
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Cesium Lead Halide perovskite (CsPbX<sub>3</sub>) perovskites have attracted attention due to their broadband absorption, narrow emissive line widths, high photoluminescence quantum yields (PLQY), and high stability. Recently, several reports stated that the electronic structure of CsPbX<sub>3</sub> can be modified and consequently the optoelectronic performance can be significantly changed by doping them with trivalent lanthanides such as (Ce<sup>3+</sup>, Sm<sup>3+</sup>, Eu<sup>3+</sup>, Tb<sup>3+</sup>, Dy<sup>3+</sup>, Er<sup>3+</sup>, and Yb<sup>3+</sup>). In particular, quantum-cutting phenomenon, when one photoexcitation creates two near-infrared (NIR) photons has been reported for Yb-doped perovskite [1,2].

To better understand the quantum cutting mechanism and properties, we have synthesized CsPbCl<sub>3</sub> perovskite doped by various content of Yb<sup>3+</sup> ions. We applied a dry synthesis technique when perovskite was synthesized by heating of carefully mixed and grinded precursor materials. With increasing the YbCl<sub>3</sub> amount in precursor mixture, the visible perovskite photoluminescence (at around 410 nm) is suppressed, and NIR emission of Yb<sup>3+</sup> ions appears. The total photoluminescence quantum yield increases from about 9% for the undoped CsPbCl<sub>3</sub> to 65% for samples doped with 5-7% concentration of Yb<sup>3+</sup>. Analysis of the VIS and NIR luminescence kinetics shows that Yb<sup>3+</sup> ions cause ultrafast quenching of perovskite excited states, while Yb<sup>3+</sup> luminescence decay kinetics strongly depends on their concentration: the relaxation time changes from about half a millisecond to almost two milliseconds when concentration of Yb<sup>3+</sup> increases from 0.5% to 9%.



**Figure 1 Atomic structure diagram of undoped (left) and Yb-doped (middle) CsPbCl<sub>3</sub> perovskite, and schematic presentation of energy transfer from perovskite to Yb<sup>3+</sup> (right)**

[1] M. Stefanski, V. Boiko, M. Ptak, W. Strek, D. R., *Alloys Compd.*, 2022, 905, 164216.

[2] Dagnall, K. A.; Conley, A. M.; Yoon, L. U.; Rajeev, H. S.; Lee, S.-H.; Choi, J. J, *ACS Omega*, 2022, 7, 20968–20974. Abstract for PSCO Oxford September 2023 Deadline 31.03.2023



# Optimization of Electron Transport Layers for p-i-n Perovskite Solar Cells

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For perovskite solar cells in inverted p-i-n structure [6, 6]-phenyl C<sub>61</sub> butyric acid methylester (PCBM) is the most common solution-based electron transport layer (ETL) due to its strong electron transport properties and relatively high electron affinity. However, it has several limitations such as poor electron mobility, difficulty in forming high-quality films, and non-ideal interface formation. Alternatively, evaporated fullerene C<sub>60</sub> is often used, which allows conformal coverage and thinner fullerene layers even on rougher perovskite layers. A second layer of bathocuproine (BCP), serving as an interlayer for band alignment adjustment, typically complements both alternatives [1].

Here, we present a detailed comparison of solution processed ETLs (PCBM and BCP) and vacuum evaporated ETLs (C<sub>60</sub> and BCP) and combinations thereof for use in opaque and semitransparent perovskite solar cells. We found that evaporated C<sub>60</sub> allows better device performance for as-grown semitransparent solar cells due to higher resilience against sputter damage. This is in agreement with a recent work by Ying et al. [2]. However, we observed that a post-deposition annealing could partially cure interface barriers. The annealing eventually leads to superior cell performance for PCBM-based devices compared to C<sub>60</sub>-based devices. Critical parameters for the BCP interface formation are the layer thickness, the sequence of dry or solution-based deposited layers, and the annealing steps after ETL deposition and after device completion. Interestingly, residual solvents in the PCBM layer were critical to achieve highly efficient semitransparent devices with PCEs up to 18.7 % and transparency > 85 % below the bandgap. In contrast, for opaque cells, a wide range of BCP layer thicknesses combined with C<sub>60</sub> lead to good cell efficiencies. In detail, we observed changes of the BCP films with a formation of local islands already after a few hours, implying an instable process and leading to locally varying layer thicknesses. However, this effect did not prove detrimental to cell efficiency and short-term stability so that a process delay after BCP and before back electrode deposition is not critical. In addition, the deposition of the back electrode seems to stop this dynamic BCP island formation – explaining why this effect seems to be overseen very often. These findings can help to improve the understanding and optimization of ETL development for opaque and especially semitransparent perovskite cells.

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[1] C. He et al., *Front. Phys.* 6 (2018), 99, <https://doi.org/10.3389/fphy.2018.00099> .

[2] Z. Ying et al, *Adv. Mater. Interfaces* 8 (2021), 2001604, <https://onlinelibrary.wiley.com/doi/10.1002/admi.202001604>

# Sublimed Fullerene for repeatable and efficient perovskite-based solar cells

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Fullerenes are near-ubiquitous in perovskite-based photovoltaics (PV) as thin-film electron selective contacts [1]. With perovskite-PV technologies now on the path towards commercialization, high-throughput deposition of fullerenes with high repeatability becomes of critical importance. Here, we report how the C<sub>60</sub> fullerene may undergo coalescence during the heating cycles associated with thermal evaporation, as shown in figure 1. Thermal evaporation is the most common technique for C<sub>60</sub> fullerene deposition. Such repeated heating is found to promote the formation of remnant fullerene derivatives with a higher molecular weight. When evaporated, these complexes are found to induce deep states within the perovskite bandgap. As a result, we find a systematic decrease in device performance when employing fullerenes that underwent an increasing numbers of evaporation cycles. This work reveals critical insights towards the industrial production of perovskite-based photovoltaic technologies and offers potential solutions such as sublimation to overcome this challenge.

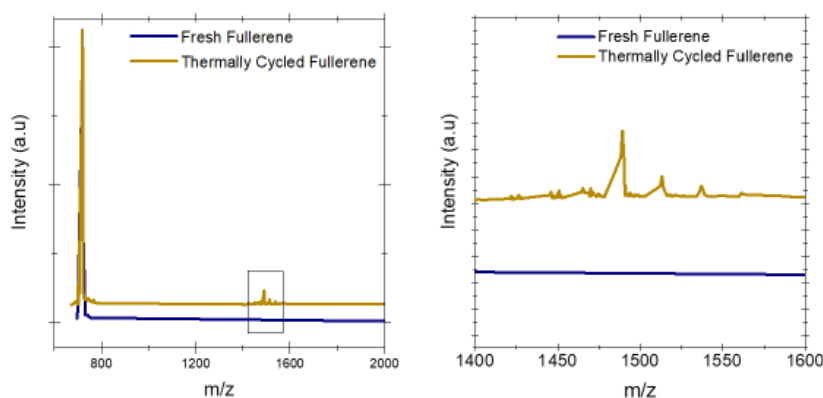


Figure 1: MALDI-TOF analysis, results for fresh and thermally cycled powders.

[1] Y. Fang, C. Bi, D. Wang, J. Huang, ACS Energy Letter (2017), 2, 782–794.

# Tailoring the Optoelectronic Properties of Tin-Based Perovskite Light-Emitting Diodes in Nonoxidative Solvent

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Two-dimensional (2D) tin-based perovskite thin films have shown tremendous potential as active materials for light-emitting diode (LED) applications, thanks to their remarkable optoelectronic properties and higher stability compared to their three-dimensional counterparts.<sup>[1]</sup> However, achieving precise control over their composition, crystallisation and morphology remains a significant challenge. To overcome these issues, a strong coordinating agent, several functionalised bulky cations, and an increasing the number of precursor materials have been applied.<sup>[2,3]</sup> Apart from that, the oxidation of Sn(II) was observed in acidic conditions under the annealing temperatures with the conventional solvent like dimethyl sulfoxide that affects the device performance dramatically.<sup>[4]</sup> In this study, we investigate the influence of additives on the growth and performance of 2D tin-based perovskite thin films in nonoxidative solvent. We employed advanced characterization techniques such as UV-Vis absorption spectroscopy, X-ray diffraction, scanning electron microscopy, and photoluminescence spectroscopy to understand its effect. By systematically varying the processing parameters, including the amount of additive and the deposition conditions, we gain insights into the underlying mechanisms governing the film formation and properties. As a result, 2D tin-based perovskite LED device had a low turn-on voltage of 1.75 V, and maximum external quantum efficiency of ~2.2% in nonoxidative solvent. The optimized thin film compositions and processing conditions from this research will facilitate the development of good performance tin-based perovskite LEDs with enhanced external quantum efficiency, and stability.

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[2] C. Liang, H. Gu, Y. Xia, Z. Wang, X. Liu, J. Xia, S. Zuo, Y. Hu, X. Gao, W. Hui, L. Chao, T. Niu, M. Fang, H. Lu, H. Dong, H. Yu, S. Chen, X. Ran, L. Song, B. Li, J. Zhang, Y. Peng, G. Shao, J. Wang, Y. Chen, G. Xing, W. Huang, *Nat. Energy* **2020**, *6*, 38.

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[4] J. Pascual, G. Nasti, M. H. Aldamasy, J. A. Smith, M. Flatken, N. Phung, D. Di Girolamo, S.-H. Turren-Cruz, M. Li, A. Dallmann, R. Avolio, A. Abate, *Mater. Adv.* **2020**, *1*, 1066.

# Achieving nearly 100% quantum-efficient lead-free perovskite solar cells with 34.67% power-conversion efficiencies through band and defect engineering-based material design optimization

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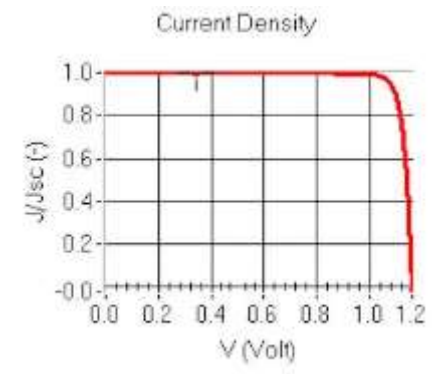
[sdajani@mit.edu](mailto:sdajani@mit.edu); [saleem.abdulfattah.aldajani@gmail.com](mailto:saleem.abdulfattah.aldajani@gmail.com); [saleem.aldajani@kaust.e-du.sa](mailto:saleem.aldajani@kaust.e-du.sa)

Perovskite-based solar cells (PSCs) have been the subject of intense research due to their high-power conversion efficiency (PCE), but their stability and lead content have limited their practical applications. In this study, we numerically simulate oxide/ perovskite/oxide-type PSCs using numerical simulations in the one-dimensional solar cell capacitance program (SCAPS-1D) [1] and Setfos [2,3] and optimize performance by tuning electronic, interfacial and defect properties. Based on these calculations, we report that a significant improvement could be achieved in the quantum and power- conversion efficiencies of a solar cell based on optimizing the design of perovskite material constituents and interfaces.

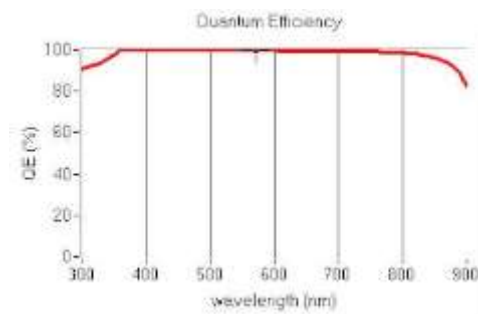
Initially, we assess the effect of various oxide-based electron transport layers (ETLs) and hole transport layers (HTLs) on PSC performance and identify a solar cell with TiO<sub>2</sub> as an ETL and NiO as an HTL (FTO/n-TiO<sub>2</sub>/CsSnI<sub>3</sub>/p-NiO) exhibiting the highest calculated PCE of 31.09%, with a fill factor (FF) of 88.43%. Next, we optimize the thickness of the TiO<sub>2</sub>, NiO, and CsSnI<sub>3</sub> layers of the benchmarked device, along with their bulk and interface defects, using detailed numerical simulations. [4, 5]

We successfully demonstrate that by engineering defects in CsSnI<sub>3</sub> and optimizing the material properties at the interface, the PCE and VOC could be further improved to 34.67% and 1.16V respectively, representing a significant jump from the initial PCE of 31.09% with a 0.98V open-circuit voltage at roughly the same FF and short-circuit current density. The specific improvements made include optimizing the band alignment of the materials to maximize light absorption, reducing the density of defects in the materials to improve charge carrier transport, and engineering the interfaces between the materials to improve charge transfer.

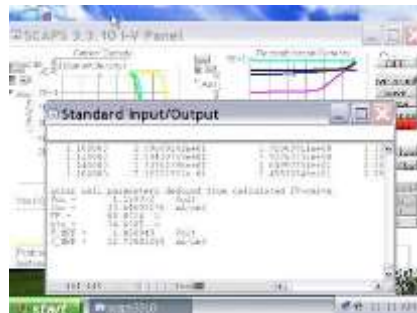
Our results provide important insights into the selection of CsSnI<sub>3</sub> as a lead-free absorber with optimized band alignment and interfacial defects, highlighting the importance of a comprehensive approach [6] to optimizing the performance of oxide/ perovskite/oxide-type solar cells that considers a range of electronic, interfacial, and defect properties. Our work demonstrates potential improvements of perovskite materials for high-efficiency solar cells. We believe that our study has significant implications for the development of practical solar cells with optimal performance based on solution-processed perovskite materials.



**Figure 1 J-V curve of perovskite solar cell with 34.67% power-conversion efficiency. Calculated using SCAPS-1D.**



**Figure 2 Perovskite solar cell exhibiting nearly 100% quantum efficiency. Calculated under 1 sun of AM1.5G irradiation.**



**Figure 3 Analysis of J-V curve for key solar performance parameters. Fill factor and short circuit current in agreement with [2].**

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# Functional P-I-N perovskite solar cell using low-damage pulsed laser deposited tin (IV) oxide electron transport layer

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In just seven years, the efficiency of halogenated perovskite on silicon tandem solar cells has risen from 23.6 % to 33.7 % on small surfaces [1], breaking the symbolic and theoretical barrier of 30 % for the simple crystalline silicon junction. The inverted P-I-N configuration of perovskite solar cells has shown significant advantages compared to the traditional N-I-P configuration, including a free-hysteresis behaviour, low-temperature fabrication process, and improved stability. As the electron transport layer (ETL), SnO<sub>2</sub> has come up as one of the most promising candidates in P-I-N tandem devices for its low-temperature compatibility, electron selectivity and broad transparency.

While recent tandem record efficiencies adopted atomic layer deposition (ALD) to grow tin oxide [2,3], this technique suffers from low deposition speeds. In this context, pulsed laser deposition (PLD) could allow large-area uniformity, reasonable deposition speed and low-damage of the underlying material.

Here we report the room temperature deposition of SnO<sub>2</sub> thin films by PLD. Their electrical and optical properties were characterised to find optimal low-damage deposition conditions. These layers were integrated as ETL of planar P-I-N perovskite solar cells. Our devices showed typical solar cell behaviour and reached a maximum power conversion efficiency (PCE) of 9.8 % under one sun illumination on a 0.13 cm<sup>2</sup> active area. While different teams have adopted the N-I-P deposition order in the past [4,5], this is to our knowledge the first demonstration of a functional ETL by PLD in P-I-N configuration.

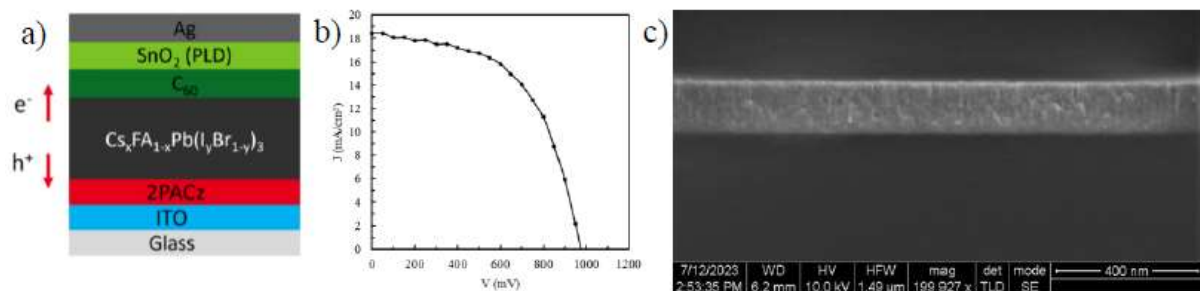


Figure 1 – a) Schematic P-I-N device, b) J-V characteristic of maximum PCE, c) SEM cross-section of SnO<sub>2</sub> deposited by PLD on Si under the integrated condition (except for a greater thickness).

[1] NREL, Best Research-Cell Efficiency Chart (2023).

[2] X. Y. Chin et al., Science (2023), vol. 381, p. 59–63.

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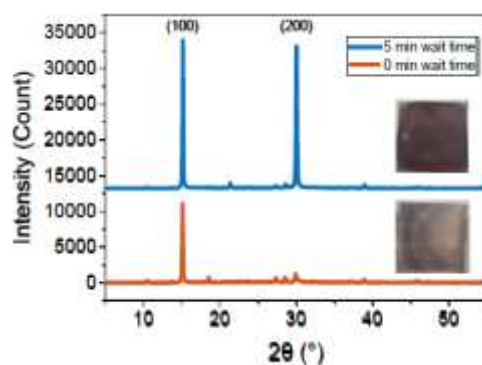
# CsPbI<sub>2</sub>Br Intermediate Phase Effect of Final Film Quality: Crystallinity, Morphology, And Phase Purity

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Inorganic Cs-based perovskites solar cells (PSCs) have attracted much attention due to their high thermal stability compared to organic-inorganic PSCs. CsPbI<sub>2</sub>Br has been especially popular among these studies thanks to its higher phase stability. Research has shown the potential of CsPbI<sub>2</sub>Br in solar cell applications; however, fewer studies focused on the impact of the intermediate phase of CsPbI<sub>2</sub>Br on its crystallisation process hence its impact on the final film quality and morphology.

In this study, we systematically investigate the impact of the intermediate phase formation on the crystallisation, phase, morphology, and crystallinity. A per-annealing wait time was introduced to assist the formation of the intermediate phase. This method has been used to control the solvent evaporation rate in an earlier study [1]. and although the study used a fixed wait time of 20 mins to improve film quality, the impact is not fully explained. For example, its impact on suppressing phase segregation, which is an unfavorable effect of lower annealing temperature crystallisation [2, 3]. The per-annealing wait time impacts the final film quality, as reflected by the X-Ray Diffraction (XRD) intensity increase. It was observed that leaving the sample at room temperature for a few minutes also suppresses the phase segregation in CsPbI<sub>2</sub>Br films. Understanding the role of the intermediate phase of CsPbI<sub>2</sub>Br on the final film, quality and phase purity is key to developing high-efficiency CsPbI<sub>2</sub>Br film.



**Figure 1 XRD results of CsPbI<sub>2</sub>Br films prepared with 0 and 5 min pre-annealing wait times.**

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# Optimization Of Wide And Narrow Bandgap Absorbers For All-Perovskite Tandem Solar Cell

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The metal halide perovskite solar cells is the fastest developing photovoltaic technology with power conversion efficiency (PCE) rising from 3.8% for a single junction solar cell in 2009 to 27.4% for all-perovskite (PK) tandem architectures in 2022 [1]. The most commonly used methods to further improve the photovoltaic performance of the PK/PK tandem solar cells include *i*) the introduction of additives into the PK material, *ii*) the PK/hole- or electron- transport interface improvement and *iii*) the charge recombination junction engineering. The present study examines the PK wide band gap/electron transport layer (PK<sub>WBG</sub>/ETL) and hole transport layer/PK narrow band gap (HTL/PK<sub>NBG</sub>) interfaces and seeks to decrease the  $V_{oc}$  losses caused by charge recombination phenomena at the interface and poor energetic band alignment.

Firstly, as regards the PK<sub>WBG</sub>/ETL interface, we study different wet and dry post- deposition PK surface treatments. We introduce an Al<sub>x</sub>O<sub>y</sub> passivation layer using Atomic Layer Deposition (ALD) and we examine the impact of the I/Br and FA/Cs ratio and morphology of the surface on the effectiveness of the Al<sub>x</sub>O<sub>y</sub> layer. Moreover, the PK/Al<sub>x</sub>O<sub>y</sub> configuration is combined with formamidinium iodide (FAI) PK-surface treatment and the effects on the PK/ETL and the photovoltaic performance are discussed. Our preliminary results show that adding the Al<sub>x</sub>O<sub>y</sub> passivation layer leads to an improved PK/ETL interface and the  $V_{oc}$  value increases by 50 mV. Combining the Al<sub>x</sub>O<sub>y</sub> layer with FAI post-PK treatment reveals that the I/Br and FA/Cs ratio at the PK surface are essential factors for the Al<sub>x</sub>O<sub>y</sub> effectiveness, since I- and FA-rich PK can negatively influence the Al<sub>x</sub>O<sub>y</sub> passivation effects and decrease the  $V_{oc}$  and Fill Factor (FF).

Secondly, we investigate the HTL/PK<sub>NBG</sub> interface and we try to replace the most commonly used poly(3,4-ethylenedioxythiophene):polystyrenesulfonate (PEDOT:PSS) HTL by : *i*) [2-(9H-Carbazol-9-yl)ethyl]phosphonic Acid (2-PACz), *ii*) methylphosphonic acid (MPA) and *iii*) 2-PACz/MPA, which are all self assembled monolayers (SAMs). Our findings show that using the PEDOT:PSS thin-film as HTL in association with a FA-cesium (Cs)-based PK<sub>NBG</sub> leads to higher  $V_{oc}$  values than the ones obtained with the SAM/PK<sub>NBG</sub> configurations, which is in contradiction to a similar study with FA-methylamonium (MA)-based PK<sub>NBG</sub> [2]. To further understand the origin of the improved PEDOT:PSS/PK<sub>NBG</sub>-based solar cell performance, the kinetics of the charge carrier recombination phenomena and the bandgap trap states of the different HTL/PK configurations are investigated using transient photoluminescence (TRPL) and ultraviolet photoelectron spectroscopy (UPS).

The optimized PK<sub>WBG</sub>/ETL and HTL/PK<sub>NBG</sub> structures are integrated in the PK/PK tandem architecture. Our preliminary results indicate  $V_{oc}$  values higher than 1850 mV and good voltage addition of the two subcells.

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# Analysis of the functionalization of ITO layers with SAMs by Inverse PES to understand

Jules Allegre

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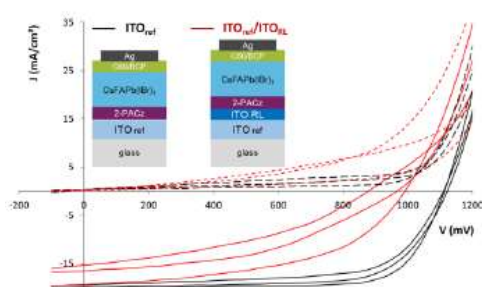
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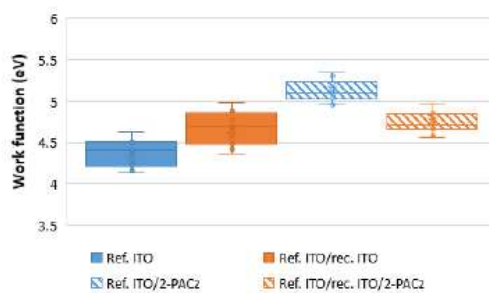
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While perovskite (PK)/silicon tandem devices continue to increase tremendously in efficiency, now exceeding the symbolic 30% limit [1], the challenge of bringing them to industrial production scale remains. In particular, the fabrication process of the PK top cell layers on large areas will require an understanding of the origin of the low shunt resistance often observed in these devices. The crucial interconnection between the two subcells in two-terminal tandem devices could play a role in mitigating shunt issues [2]. At INES, a thin ITO recombination layer (ITORL) ensures this interconnection. It has been observed that this layer has a major impact on the shunt behaviour of the top cell. For example, when fabricating single junction PK cells based on the top cell stack used in tandems, cells made on a commercial reference glass/ITO substrate (ITOfref) show comparable and satisfying performance, and no shunting. However, the introduction of the ITORL used in tandems on top of the ITOfref causes strong shunts, affecting not only the fill factor but also the open circuit voltage of the devices (Fig.1).

Phosphonic acid (PA) hole transport self-assembled molecules (HT SAMs), such as 2-PACz, increase the work function (Wf) of the ITO surface when anchoring their PA group on it [3], pushing the ionization potential (Ip) of the stack close to the perovskite valence band edge energy, which is desirable for a good hole-selective contact [4]. We analyzed the Wf/Ip of different ITO and ITO/2-PACz stacks in an Inverse Photoemission Spectroscopy (IPES) setup (Fig.2). While the 2-PACz anchoring on the ITOfref indeed results in a significant increase of its Wf, this is not the case for the ITOfref/ITORL stack. This could explain a reduced ability of the ITOfref/ITORL/2-PACz stack to repel electrons, resulting in the decreased shunt resistance and VOC observed in the devices.



**Figure 1** J(V) curves (plain: illuminated, dashed: dark) of 0.33 cm<sup>2</sup> PK solar cells made on different ITO stacks.



**Figure 2** Work function of different ITO and ITO/2-PACz stacks measured in the IPES setup.

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# Unveiling the Degradation Mechanism of Hybrid Tin-Lead Perovskites

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Organic-inorganic metal halide perovskites are a promising class of photovoltaic materials due to their exceptional efficiency and cost-effectiveness. However, their practical use is hindered by the inherent instability of the material, which leads to a short lifespan of the devices they power. Mixed tin-lead perovskites offer unique optoelectronic features, including small bandgaps ( $<1.3$  eV), making them useful for various applications (tandems, NIR light detection, and imaging e.g.). Still, the low ambient stability of tin-lead perovskites obstructs their scale-up, necessitating extensive research into their underlying breakdown mechanisms. This study aims to better understand these mechanisms and the involvement of halide chemistry, specifically emphasizing the significant role of iodine in perovskite deterioration. Our findings reveal that tin-lead-based perovskites experience cyclic degradation, with iodine and SnI<sub>4</sub> as key degradation products that harm the stability of the perovskite. Investigating the impact of iodine is critical because it is a common component of the perovskite material, and its presence has been shown to play a crucial role in the optoelectronic properties of the perovskite. Therefore, understanding the role of iodine in perovskite deterioration is essential to improve the stability and durability of tin-lead perovskites and bring them closer to commercialization. By gaining insight into the degradation mechanisms of tin-lead perovskites, we can develop effective strategies to mitigate their degradation, enhance their stability and lifespan, and unlock their full potential for use in various photovoltaic applications, contributing to a more sustainable and environmentally conscious future.

# Quantifying Defects in CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> Perovskite Solar Cells using Capacitance Spectroscopy Techniques

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Metal halide perovskites have gained immense attention from photovoltaic research community due to its phenomenal optoelectronic properties that has skyrocketed the power conversion efficiency (PCE) of perovskite solar cells to 25.7% over the past decades [1]. The research scientists have endeavoured to provide insights on the device physics of perovskite solar cells (PSC). Special attention is required to comprehend the details governing the role of defects and its properties on the performance of PSCs. Defects in the bandgap or at its interfaces in perovskite elicit anomalous behaviour of the performance as it acts as a recombination centres and ion migration sites. To probe the defect properties, we have explored capacitance measurement approach such as capacitance-voltage (CV), capacitance-frequency (C-f), thermal admittance spectroscopy (TAS) and deep-level transient spectroscopy (DLTS) to quantify the defect properties in CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> based perovskite solar cells [2,3]. The steady-state capacitance vs frequency scans at different temperatures (C-f-T) from 200K to 350K reveal three capacitance steps at low frequency-high temperature, high frequency-low temperature and at intermediate frequency and temperature. The voltage dependent (C- f-T) allows to distinguish the surface and bulk defects. The low frequency capacitance shows prominent increase in capacitance with increase in temperature due to ionic contribution. The prominent defects were observed with activation energies of 0.16eV and 0.54eV from the band edges. However, the nature of traps can be determined using transient capacitance technique. The capacitance transient spectra at different temperature (C-t-T) from 200K to 350K shows anomalous behaviour such as capacitance increases initially with temperature and then decreases above 320K possibly due to perovskite phase transition. DLTS measurements reveal a dominant defect level with activation energy of 0.56eV. These findings show qualitative agreement with the theoretical values using DFT calculations reported in literature. Eventually, we provide comprehensive insights into charge accumulation, band bending and capture and emission process using band diagrams.

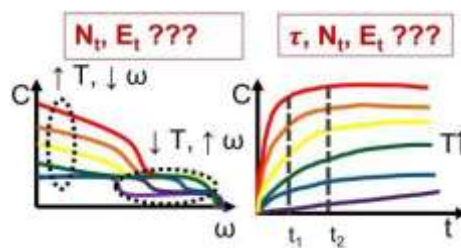


Figure 1 Illustrates the capacitance-based approach to probe the defect properties.

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# Enhanced optoelectronic coupling for monolithic perovskite/silicon tandem solar cells

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Monolithic perovskite/silicon tandem solar cells are of great appeal as they promise high power conversion efficiencies (PCEs) at affordable cost. In state-of-the-art tandems, the perovskite top cell is electrically coupled to a silicon heterojunction bottom cell via a self-assembled monolayer (SAM), anchored on a transparent conductive oxide (TCO), enabling efficient charge transfer between the subcells. Yet, reproducible high-performance tandem solar cells require energetically homogenous SAM coverage, which remains challenging, especially on textured silicon bottom cells. Here, we resolve this issue by developing new TCOs that serve interconnecting layers, resulting in high surface-potential homogeneity and higher density of SAM anchoring sites when compared to commonly employed crystalline TCOs. Combined with optical enhancements at the front and rear electrodes, an independently certified PCE of 32.5% was obtained, which ranks amongst the highest for perovskite/silicon tandems

# The Effect of Antimony Substitution on the Optoelectronic Properties of MAPbI<sub>3</sub>

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The long-term stability of metal halide perovskites has been a consistent concern halting their commercialisation. Chemical substitution of the A (cation) and X (halide) sites have garnered attention due to its ability to improve stability and tune the optoelectronic properties of metal halide perovskites [1]. However, a less explored route is B-site substitution, especially using heterovalent metals. With concerns surrounding lead toxicity, the development of lead-free metal halide perovskite alternatives is also growing in interest [2]. However, previous studies have shown that heterovalent doping has an adverse effect on its optoelectronic properties [3], emphasising the importance of understanding the effect of these heterovalent metals on the charge-carrier dynamics and optoelectronic properties in metal halide perovskites. In this work, we study the optoelectronic properties of MAPbI<sub>3</sub> substituted with antimony with the general formula MAPb<sub>(1-x)</sub>Sb<sub>x</sub>I<sub>(3+x)</sub> (MAPbI<sub>3</sub>-Sb, where x = 0, 1, 5, 10 %) using a combination of photoluminescence (PL), time-resolved PL (TR-PL) and optical-pump/THz-probe (OPTP) spectroscopy. We observe a decrease in PL intensity and charge-carrier lifetime with increasing antimony substitution, attributed to an increase in trap sites. With OPTP measurements, this work also reveals decreased charge-carrier mobility with increasing antimony substitution which is linked to enhanced impurity scattering.

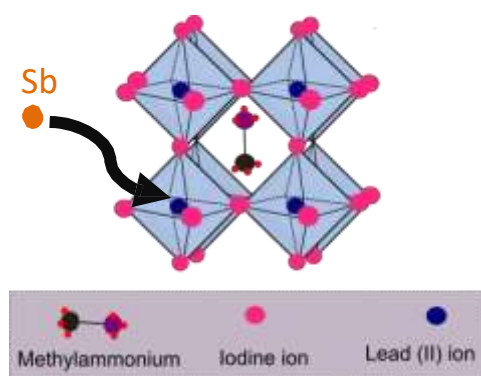


Figure 1 Antimony B site substitution of MAPbI<sub>3</sub>.

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# An underwater city solar: high-band gap bromide-based perovskite solar cells for underwater application

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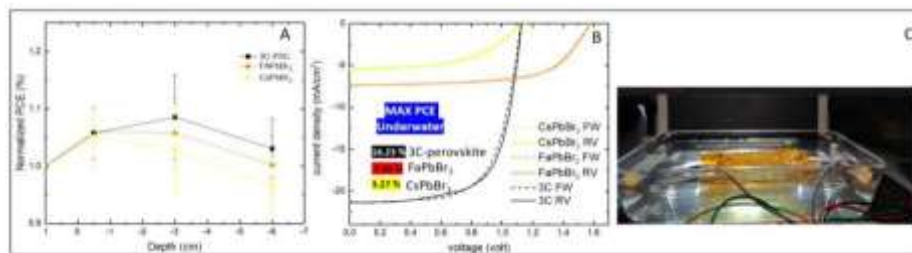
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In a time of energy crisis, the need to differently develop the energy system of our territory drives us to explore different solution and application. The underwater (UW) environment is part of our daily life considering sportive activities in swimming pools, business enterprise such as fish farming and educational activities in aquariums. Besides BIPV and roof top's application, PV devices can be utilized in the agrivoltaic field, in the space but the underwater environment is still unexploited. When the depth increases, highest wavelengths are absorbed and at depth of 50 meters the blue-green light from 400 to 600 nm is present. Recently, theory analysis calculated that ideal candidate for UW application at deep depth are high band gap (2-2.2 eV) devices [1]. In this work, we aim to present a pioneering experimental application of two high-bang gap perovskite solar cells, semi-transparent and bifacial devices, FaPbBr<sub>3</sub> and CsPbBr<sub>3</sub>, comparing them with a reference triple-cations perovskite solar cell. With a transparent and robust encapsulant, we challenged the perovskite's sensitive in a humid environment, testing the three devices at depth of -1 cm, -3 and -6 cm from the water surface. Moreover, we merge experimental results with theoretical ones pushing the limit to -5 meter.



**Figure 1** A) PCE trend underwater (UW) for reference cell 3C perovskite, FaPbBr<sub>3</sub> and CsPbBr<sub>3</sub>. B) J-V of maximum PCE UW. Active are of 1 cm<sup>2</sup>. C) FaPbBr<sub>3</sub>-based module tested UW

By measuring devices just below the waterline, their conversion efficiency increases due to the different refraction index of water, moreover the cell's overheating problem is overcome due to the cooling of the water. This may be a room of discussion with the aim to consider a new neutral-land energy's production system.

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# Charge Localization in $\text{Cs}_2\text{AgBiBr}_6$ Halide Double Perovskite: Small Polarons and Self-Trapped Excitons

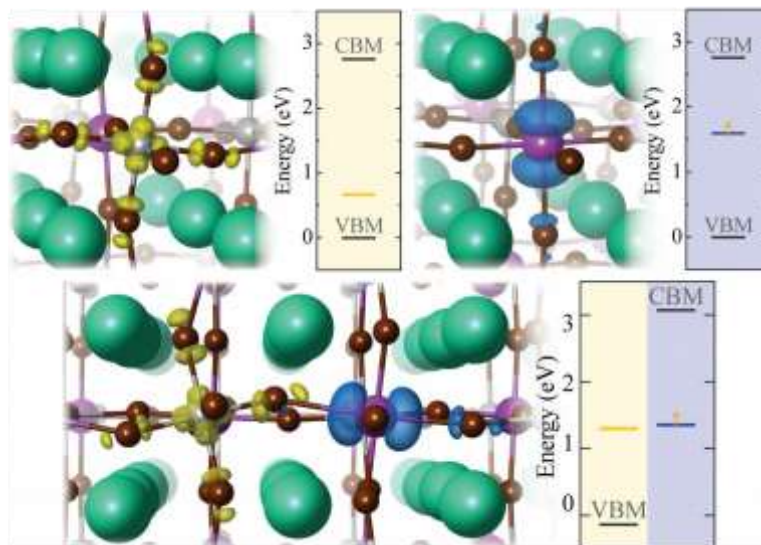
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Halide double perovskites have gained vast interest in optoelectronic applications. Their relatively soft crystal lattice structure allows deformations that can trap charge carriers, leading to the formation of small-polaron states. Therefore, small-polarons can play an essential role in charge carrier transport in halide double perovskites, and it is important to develop theoretical models that can accurately predict the behavior of polarons in these materials. In this study, we investigate hole and electron polarons in  $\text{Cs}_2\text{AgBiBr}_6$ , a widely-studied halide double perovskite, using the hybrid PBE0( $\alpha$ ) functional that satisfies the Koopmans' condition. Our results demonstrate that an excess electron localizes on the Bi atom, while an excess hole localizes on the Ag atom. The impact of spin-orbit coupling (SOC) is found to be significant and must be considered for accurate modeling of polarons in  $\text{Cs}_2\text{AgBiBr}_6$ . In addition, co-localization of holes and electrons at close proximity Ag and Bi sites is explored, and it is found that there is a significant attraction between the two types of polarons, leading to the formation of triplet self-trapped excitons (STEs). Our results provide insights into the essential properties of  $\text{Cs}_2\text{AgBiBr}_6$  and have potential implications for the development of green devices based on this material.



**Figure 1: Isosurfaces of hole and electron polarons, as well as self-trapped exciton, with corresponding energy levels for the localized charges.**

# Sequentially hybrid vacuum-processed Multi-Cation Halide Perovskite

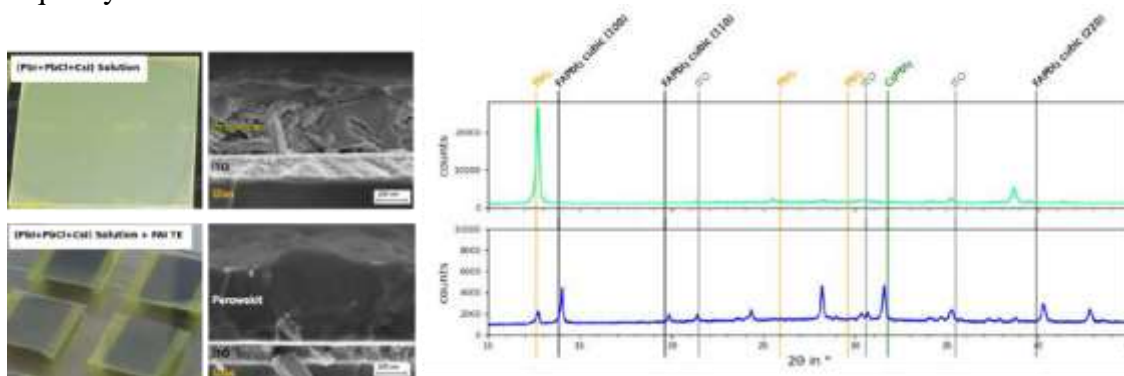
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Multi-cation halide perovskite is considered to be a highly promising solar cell material. Going from solution-based perovskite deposition to thermal evaporation leads to several advantages as conformal coverage and good control over film thickness and uniformity, also reflected in the widespread use of thermal evaporation in the semiconductor industry [1]. However, we report on the interesting combination of a hybrid sequential deposition method consisting of a solution-based deposition of a lead containing precursor followed by vacuum deposition of formamidinium (FAI) to get a FACsPbI<sub>3</sub>-perovskite film after thermal annealing which was recently reported to have the potential of very efficient and robust perovskite layers [2]. The Cs-component was either directly included in the precursor solution or sequentially evaporated before the FAI evaporation with distinct differences in film quality formation.



**Figure 1:** hybrid deposition method with Cs-containing precursor solution, top row: only precursor bottom row: with subsequently evaporated FAI, from left to right: Image, SEM cross section image, XRD data.

From the X-ray diffraction data of Figure 1, one can see a reduced PbI<sub>2</sub>-Peak at 12.6° after the deposition of FAI and the subsequent annealing step. Moreover, the FAPbI<sub>3</sub>- (100)-Peak appears at 13.85° so that it can be concluded that the crystallization to the cubic  $\alpha$ -phase perovskite has taken place. With this knowledge, we have already built a functioning full solar cell stack in inverted p-i-n architecture. More details of process variations and its influence on film and device properties will be discussed.

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# Scalable Perovskite Top Cells for Monolithic PSTSCs

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As means to surpass the efficiency limitations of silicon technology, perovskite/silicon tandem solar cells (PSTSC) have increasingly gained focus of companies and research institutes alike. Recent efficiency records of 32.5% [1] using lab processes establish the potential of this technology, but also highlight the need to address the efficiency gap to large area PSTSCs, while keeping production costs low. Furthermore, textured surfaces of state-of-the-art industrial Czochralski-based silicon bottom cells pose additional challenges for wet deposition techniques predominantly used in the fabrication of perovskite devices. Thermal co-evaporation as a dry-vacuum method, has already achieved 24,6 % efficiency [2]. It features conformal and homogenous coverage of large areas and could be utilized to bring perovskite to industrial scales. To demonstrate the viability of fully vacuum processed perovskite top cells on industrial silicon solar cells, HZB has formed a collaboration with the companies *von Ardenne* and *CreaPhys* to develop a cluster tool which can process fully functional co-evaporated perovskite top cells on large (Substrate sizes of 166×166 mm<sup>2</sup> (M6), but up to 182×182mm<sup>2</sup> (M10) is possible), without breach of vacuum. The tool is equipped with two evaporators, an ALD and two sputter chambers, which enables the fully automatic production of 12 M6- size substrates into functioning PSTSCs. This work focuses the perovskite MAFAPbI<sub>3</sub>, which offers decent stability and has been shown to conformally cover TaTm as hole transport layer, thereby yielding high open-circuit voltages and fill factors. With this, a tandem device with an efficiency of 22.45% under standard AM1.5G conditions (see Figure 1) could be demonstrated.

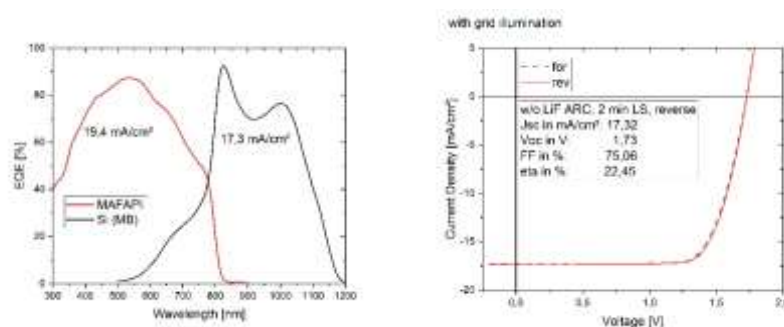


Figure 1: A) external quantum efficiency and B) JV curve of a PSTSC with MAFAPbI<sub>3</sub> top cell absorber.

[1] Best Research-Cell Efficiency Chart, NREL, accessed 01.02.2023, <<https://www.nrel.gov/pv>>

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[3] A. Al-Ashouri et al., Science (2020), 370, 1300

# Passivation of defects in perovskite solar cell using Enamine Analogue of Tetra-Phenylethylene: A New Systematic Pathway to Achieve High Performance

Shubhangi Bhardwai<sup>1</sup>

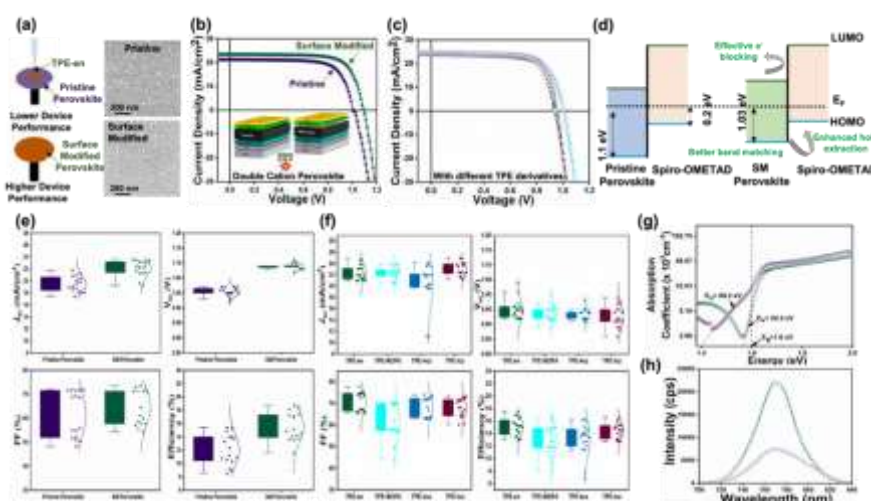
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In this work we demonstrate the use of a novel enamine derivative of tetra phenylethylene (TPE-en) organic material to reduce the interface defects which enhances the performance of perovskite solar cells (PSCs). The introduction of TPE-en at the surface of the perovskite (PSK) film resulted in 23% reduction in the champion device's ideality factor, drop in leakage current, and 8-13% improvements in the device's short-circuit current density, 2-8% in fill factor, and ~80 meV in open circuit voltage. The total power conversion efficiency achieved was 18.73% (with double cation surface modified (SM) PSK, a 3% improvement over pristine PSK-based solar cells. We also obtained similar improvement in case of triple cation-based SM PSK with 21.61% champion cell efficiency. ss-PL and TRPL shows 3 times improvement in PL intensity and carrier lifetime respectively. Urbach energy indicate a drop of 67 meV in sub-band gap region. Thus, SM PSK exhibited reduced surface defects, attenuated non-radiative carrier recombination, higher carrier lifetimes and a significant reduction in trap centres in the sub band gap region. XPS showed there is no band bending and thus, no field effect passivation. UPS studies revealed effective band alignment in case of SM PSK in comparison to pristine with SPIRO-OMETAD, resulting in improved hole extraction and enhanced photovoltaic performance. On comparison, TPE-en-based device outperformed other reported TPE derivatives like TPE-MDPA, TPE-4Cz, TPE-tcz.



**Figure 1** (a) Scheme illustration and FESEM image, (b, c) Light J-V characteristics of the champion cells, and (e, f) Statistics of J<sub>sc</sub>, V<sub>oc</sub>, FF, and PCE using pristine and surface modified PSK with different TPE derivatives as absorber layer, (d) band alignment at the interface of PSK and hole transport layer, (g) absorption coefficient and (h) PL of pristine (in purple) and SM PSK (in green) respectively

# Scaling of Perovskite Silicon Tandem Solar Cells – Progress and Challenges

Juliane Borchert<sup>1,2</sup>

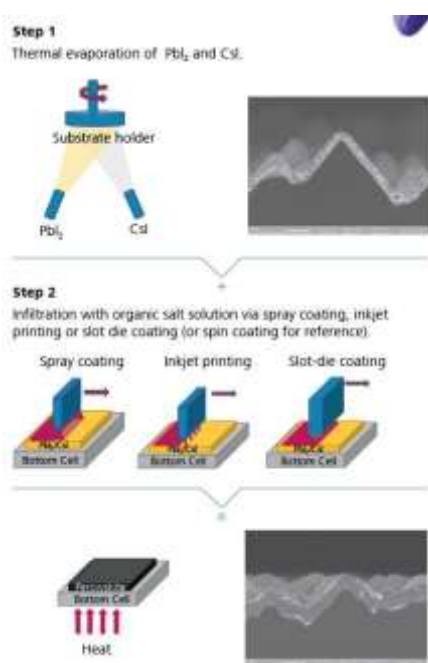
Oliver Schultz-Wittmann,<sup>1</sup> Patricia S. C. Schulze,<sup>1</sup> Oussama Er-Raji,<sup>1,2</sup> Bhushan Kore,<sup>1,2</sup> Raphael Efinger,<sup>1</sup> Ulrike Heitmann,<sup>1</sup> Markus Kohlstädt,<sup>1</sup> Sebastian Pingel,<sup>1</sup> Timo Wenzel,<sup>1</sup> Henning Nagel,<sup>1</sup> Martin Bivour,<sup>1</sup> Martin Hermle,<sup>1</sup> Stefan W. Glunz<sup>1,2</sup>

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Perovskite-silicon tandem solar cells are a highly promising technology for the next generation of solar cells. These tandems should be textured on the front and the rear side to maximize energy yield under field conditions [1]. Since the standard lab procedure of wet-chemical spin coating does not yield conformal coating on  $\mu\text{m}$ -sized textured surfaces, we use a **two-step hybrid route** to deposit mixed cation mixed halide perovskite absorber films [2]. In a first step, the inorganic components are thermally evaporated to form a scaffold, allowing for conformal coating of random pyramid textured silicon. In a second step, the conversion into perovskite is accomplished using a solution containing the organic components. A thermal anneal completes the conversion to a polycrystalline perovskite layer. For the second step, we evaluate several deposition techniques which are already used in other industrial fields: a) spray coating b) ink jetting c) blade coating d) and spin coating as a reference process. To enable the scaling and industrial use of perovskite-silicon solar cells it is crucial to understand and control the physical and chemical processes happening during the deposition of the perovskite films



and adjacent contact layers. In this contribution we present our efforts to upscale perovskite-silicon tandem solar cells from small solar cells that are embedded in larger area substrates to full wafer area devices. We have integrated a printed front electrode and are currently processing full area 100x100 mm<sup>2</sup> wafers as an intermediate step towards industrial wafer size areas. We have successfully applied the hybrid route on textured silicon bottom cells to provide conformal coatings using scalable technologies. While significant progress has been made, challenges remain that need to be overcome to make highly efficient perovskite silicon solar cells ready for fabrication on an industrial scale.

**Figure 1** To process perovskite films onto textured silicon we follow the hybrid deposition route.

[1] N. Tucher, et al. "Energy yield analysis of textured perovskite silicon tandem solar cells and modules," Opt. Express 27,A1419-A1430,(2019), doi:10.1364/OE.27.0A1419

[2] Patricia S.C. Schulze, et al., "Perovskite hybrid evaporation/ spin coating method: From band gap tuning to thin film deposition on textures", Thin Solid Films, Volume 704, 2020, doi: 10.1016/j.tsf.2020.137970

# Bifacial Module for 4-Terminal Hybrid Tandem

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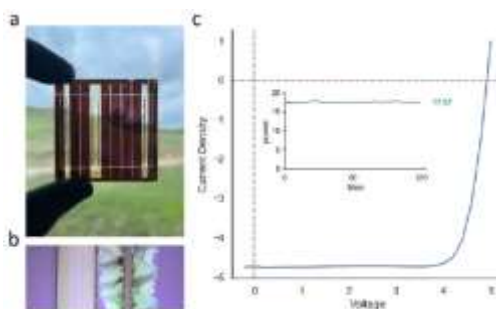
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While scaling perovskite technologies to manufacturing and distribution, many have set their sights on tandem architectures. Four terminal (4T) hybrid tandem devices potentially ease integration of perovskites with existing solar technologies, such as Silicon and CdTe. Such 4T tandem devices will need two transparent contacts. The most common back contact Transparent Conducting Oxides (TCO) are Indium Tin Oxide (ITO) or Indium Zinc Oxide (IZO). ITO requires high temperatures to achieve the crystallinity necessary for relatively high conductivity and transparency. IZO may be deposited at room temperature and is amorphous. However, transparent conductive oxides like ITO and IZO complicate monolithic module scribing, where one must isolate neighboring cells using P1 and P3 scribes and establish cell-to-cell interconnects using P2 scribes. The TCO contacts are thicker than metallic contacts, and they are necessarily transparent to visible and near-infrared light. In this case, the transparency of the TCO to visible and near-infrared frequencies means that it is more difficult to ablate it directly using a laser. Instead, the laser is preferentially absorbed in the perovskite layers beneath the TCO, which produces a shock wave that causes the TCO to erupt at the edges of the P3 scribe. This eruption can cause TCO lift-off that extends for hundreds of micrometers, potentially reducing achievable geometric fill factors (GFF). In the long run, adhesion issues in the stack and inherent stresses in the TCO can cause it to delaminate entirely in the field, starting at the damaged P3 edge [1]. At the P2 scribe interconnect, using TCO instead of metal contacts protects the scribe-exposed stack against halide-metal interactions [2-4]. However, because TCOs are far more resistive than metal contacts, it is more difficult to establish low resistance and high-GFF P2 interconnects. In this work, we address difficulties associated with the P2 and P3 scribes in a bifacial, all-TCO module. We report on efforts to adjust geometric fill factor, to adjust the TCO deposition process parameters to reduce stress, and to use additional interlayers that promote adhesion or otherwise protect the stack from laser-induced damage. We then demonstrate >17% zero-albedo bifacial perovskite modules using a wide-bandgap perovskite absorber, suitable for 4T silicon-perovskite tandem applications, which we encapsulate and test outdoors.

**Figure1: a) complete bifacial module whose scribes and JV data follow.**

**b) optical microscope images of P1, P2, and P3 scribes, including delamination from P3 scribe. c) JV curve from 6.5cm<sup>2</sup> bifacial module, with MPPT inlay.**



[1] Mukesh Kumar, A.K. Sigdel, T. Gennett, J.J. Berry, J.D. Perkins, D.S. Ginley, C.E. Packard, *Applied Surface Science* (2013), 283, pg 65-73 (<https://doi.org/10.1016/j.apsusc.2013.06.019>)

[2] R.A. Kerner, P.Schulz, J.A. Christians, S.P. Dunfield, B. Dou, L. Zhao, Gl. Teeter, J. Berry, B. P. Rand et al, *APL Mater* (2019), 7, 041103.

[3] R.A. Kerner, L.F. Zhao, S. P. Harvey, J. J. Berry, J. Schwartz, and B.P. Rand, *ACS Energy Lett* (2020), 5, 3352-3356.

[4] R.A. Kerner, A.V. Cohen, Z. Xu, A.R. Kirmani, S.Y. Park, S.P. Harvey, J.P. Murphy, R.C. Cawthorn, N.C. Giebink, J.M. Luther, K. Zhu, J.J. Berry, L. Kronik, B.P. Rand, *Adv Mater* (2023),

# Unraveling the Mysteries of Potential-Induced Degradation: A Precise Method for Revealing Critical Insights on Perovskite Solar Cells

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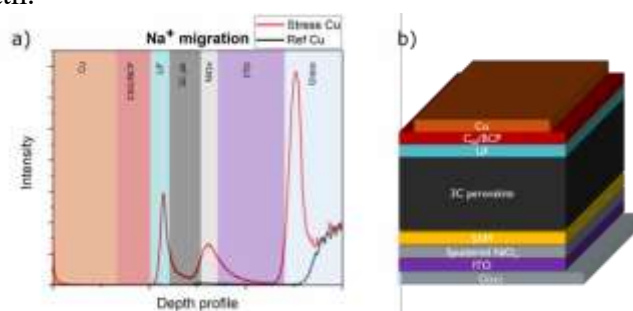
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Potential-induced degradation (PID) is a severe photovoltaic (PV) system-related degradation mechanism and one of the major reliability issues in commercial solar cells [1]. Recent studies demonstrated almost complete degradation in only 18 hours of PID- stress testing [2,3]. Perovskite solar cells (PSCs) are sensitive to light, moisture, and thermal stress. Therefore, the unintentional occurrence of other degradation mechanisms is possible, making it challenging to isolate the PID effect in ambient conditions at elevated temperatures. This research is the first to report on PID-stress tests at room temperature in a controlled nitrogen environment. Consequently, the exclusion of other degradation mechanisms can be ensured to a high degree, providing accurate insights into PID. Stress tests were conducted on triple-cation p-i-n PSCs using the foil method, described in IEC 62804-1, at 25°C and 1000V potential difference for over a week. To gain first insights, the sensitivities of PSCs contacted with copper and indium tin oxide to PID were compared, and it could be observed that the latter samples are less susceptible. In addition, figure 1 presents Time-of-Flight Secondary Ion Mass Spectroscopy (ToF- SIMS) measurements that provide evidence of sodium ion migration from the front cover glass through the perovskite layer, reducing the device performance. Additional experiments on diverse device architectures will provide crucial insights into the sensitivity to PID. Ultimately, these insights will be critical in devising effective PID- mitigation strategies and developing more stable PSCs under operating conditions, which can accelerate their commercialization path.



**Figure 1: (a) ToF-SIMS analysis indicating sodium migration in a copper-contacted sample and (b) a graphical representation of the stack utilized in this research.**

[1]W. Luo, Y. S. Khoo, P. Hacke, et al., *Energy and Environmental Science* 2017, vol. 10, no. 1., pp. 43–68

[2]Z. Purohit, W. Song, J. Carolus, *Solar RRL* (2021), vol. 5, no.9, p. 2100349

[3]J. Carolus, T. Merckx, Z. Purohit, *Solar RRL* (2019), vol. 3, no. 10, p.1900226

# Distinguishing Carrier Transfer and Recombination at Perovskite-Transport Layer Interfaces Using Time-Resolved Spectroscopy

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In a perovskite solar cell, photovoltaic action arises due to the heterojunctions formed by the perovskite layer and the charge transport layers (CTLs) on either side. As the fabrication of high-quality thin films of metal halide perovskite matures, the optimisation of these charge transport layers and their interfaces becomes increasingly important [1]. In this work, the electrical properties of these heterojunctions were studied by time-resolved optical measurements of the charge carrier dynamics in perovskite-CTL bilayers.

Bilayers were formed by depositing the electron transport layers (ETLs) PCBM and C60, or the hole transport layer (HTL) Spiro-OMeTAD, on top of a triple cation [2] perovskite layer (FA<sub>0.79</sub>MA<sub>0.16</sub>CS<sub>0.05</sub>)Pb(I<sub>0.83</sub>Br<sub>0.17</sub>)<sub>3</sub>. Time-resolved terahertz (THz) photoconductivity and transient absorption (TA) spectroscopies were used to track the photoexcited carrier population in the perovskite from femtosecond to nanosecond timescales, whilst time resolved photoluminescence (TRPL) followed the population decay on nanosecond to microsecond timescales.

The measured carrier dynamics were compared to numerical simulations of the carrier density, that included the Poisson equation to account for charge separation across the interface, which is usually ignored. The numerical simulation revealed that the desired charge separation should leave a characteristic fingerprint in the decay curve, and its absence indicates fast interfacial recombination. This analysis can be applied to study any CTL, and here it showed that despite their high performance in devices, PCBM and C60 layers have significant interface recombination on sub-nanosecond timescales. Spiro-OMeTAD on the other hand benefits from much slower interface recombination, but hole extraction is also much slower. Interface recombination and ambipolar diffusion coefficients were extracted by fitting the model to the data, and simultaneously fitting decay curves for different initial distributions of carriers provided tighter constraints.

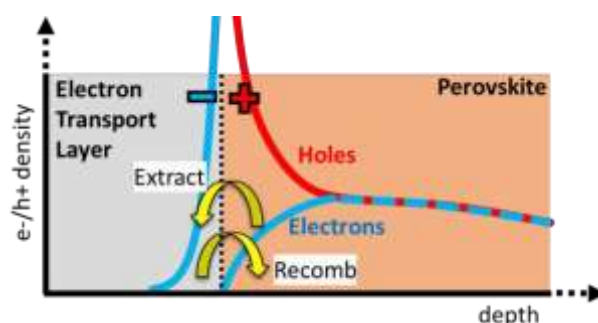


Figure 1 Schematic of charge separation across a perovskite-CTL interface.

[1] P. Schulz, D. Cahen, and A. Kahn, *Chemical Reviews* (2019), 119, 3349–3417.

[2] M. Saliba et al., *Energy and Environmental Science* (2016), 9, 1989–1997

# How to get over 25.5mA cm<sup>-2</sup> integrated current density in perovskite solar cells and modules: substrate choice, annealing, additives and passivation strategies investigation

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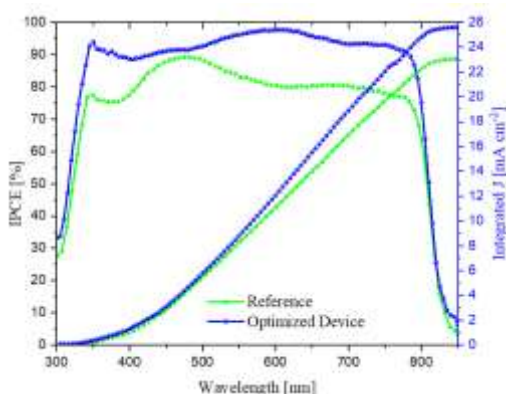
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Perovskite Solar Technology is coming to a turning point, with efficiencies reaching up to 25.7%<sup>[1]</sup>. These results are obtained on FAPbI<sub>3</sub> based perovskite and only by few research centres worldwide, mainly due to a well-known narrow band-gap perovskite structure difficult to stabilize<sup>[2][3]</sup>. In this work, FAPbI<sub>3</sub> based perovskite have been investigated under different strategies: firstly, a comparison of the substrate and transparent conductive oxides allows to absorb more current mainly in the UV region (Figure 1); secondly, a study on different annealing temperature revealed that the perovskite grains and phase are temperature sensible, with  $\alpha$  to  $\delta$ -phase reversible transition below 120°C. Moreover, the use of additives in the perovskite precursors, already shown in our previous work<sup>[4]</sup>, but also others, such as methylammonium chloride (MACl) and phenethylammonium iodide (PEAI), allows a further current improvement, but mainly shown an overall improvement on the open circuit voltage (Voc) of the device. Finally, the use of a capping layer over perovskite film, such as phenethylammonium chloride and others 2D perovskite precursors, showed an overall improvement of the final power conversion efficiency (PCE) of devices, with a remarkable enhancement of the integrated current density, showing an improvement from 23.11mA cm<sup>-2</sup> to 25.59mA cm<sup>-2</sup>. These optimization have been used for both flexible and upscalable devices, reaching highly efficient devices on micro modules size, with an active area of 2.5cm<sup>2</sup>. This work could be helpful to both research community and industries, to raise the bar of the perovskite single junction state of the art, bringing simple and helpful information to anybody.



**Figure 1** Incident photon to converted electrons [IPCE] of the reference (green dots) and optimized device (blue dots). The calculated integrated current density is 23.11mA cm<sup>-1</sup> and 25.59 mA cm<sup>-1</sup> for the reference and optimized device, respectively.

[1] J. Park, J. Kim et al. *Nature* (2023) doi:10.1038/s41586-023-05825-y [2] W. Peng, K. Mao et al. *Science* (2023) 379, 6633.

[3] H. Yun, H.W. Kwon et al. *Nature Energy* (2022) 7, 828-834.

[4] L.A. Castriotta, E. Calabrò et al. *Nano Energy* (2023) 109, 108268.

# New insights for developing lower-toxicity and stable inkjet-printable perovskite precursor inks for fully-printed annealing-free perovskite PVs manufacturing

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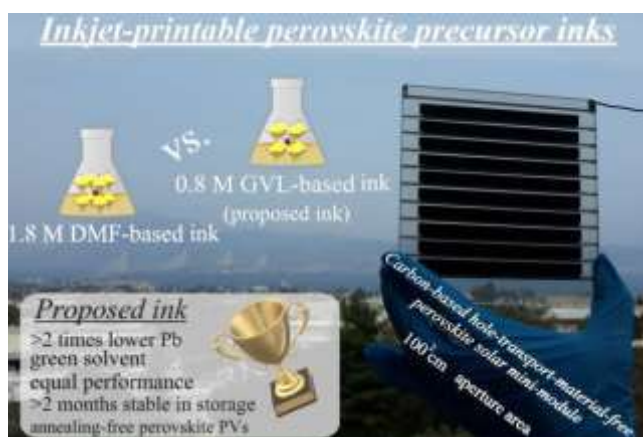
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Piezoelectric drop-on-demand inkjet-printing is considered an emerging manufacturing process for the development of perovskite solar cells (PSCs) with low material waste and high production throughput. Until now, all case studies focused on inkjet-printed PSCs have relied on the use of hazardous solvents and/or high-molarity perovskite precursor inks, both of which are known to enable the development of high-efficiency photovoltaics (PVs). The work presented herein provides a new insight for the development of lower-toxicity, high-performance and stable (for more than two months in storage) inkjet-printable perovskite precursor inks for fully ambient air processed PSCs. The capability of producing high-quality and with minimum coffee-ring defects, annealing-free perovskite absorbent layers under ambient atmosphere conditions is demonstrated using an ink composed of a green low vapor pressure noncoordinating solvent and only 0.8 M of perovskite precursors (more than 2 times lower than the usually applied concentration (see **Figure 1**)). Notably, the PSCs manufactured utilizing the industry-compatible carbon-based hole transport material free design and the proposed ink attain >13% efficiency, which is considered on the performance records for the under-consideration PV architecture employing an inkjet-printed active layer. Outstanding is also the stability of the PV devices under the conditions specified by the ISOS-D-1 protocol ( $T_{95} = 1000$  h). Finally, the scaling up of the solar cell devices to the mini-module level (100 cm<sup>2</sup> aperture area) is demonstrated, with the upscaling losses to be as low as 8.3%rel dec<sup>-1</sup> per upscaled active area.



**Figure 1** Gamma-Valerolactone as a green solvent alternative for the development of lower-toxicity and stable inkjet-printable perovskite precursor inks for all-printed annealing-free perovskite photovoltaics.



# Cesium Tin Halide based Absorber Layers for Graphene-derived all- inorganic Flexible Perovskite Solar Cells

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The growing energy need and rapid consumption of conventional energy resources motivated researchers to find feasible and cheap alternative resources. The wafer-based crystalline silicon photovoltaics is a commonly used solar cell technology, but it has high-cost and limited stock. Nowadays, perovskite solar cells (PSCs) have emerged as promising next-generation photovoltaic technology due to their low cost. A remarkable power conversion efficiency (25.7%) has been demonstrated for organic-based PSCs [1]. Still, these are most degradable and less stable as the performance degrades rapidly because these perovskite materials decompose under ambient conditions [2]. Therefore, the instability of perovskites is a significant challenge in commercializing this solar cell technology. Since different solvent and material engineering can tailor the material properties and power-conversion efficiency, a study on the metal oxide-based all- inorganic CsSnI<sub>3</sub>Cl<sub>3-x</sub> layers is explored herein for flexible PSCs. In different processing conditions, the microstructural and optical properties are optimized to enhance the stability and performance of metal oxide-based ecofriendly flexible PSCs. Alumina is used as an efficient scaffold layer, which engineers CsSnI<sub>3</sub>Cl<sub>3-x</sub> halide perovskite material to attain efficient charge transport and long-term stability. We hope to achieve considerably enhanced stability of high-efficiency eco-friendly flexible perovskite solar cells.

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[1] S. Chander et al., Mater. Sci. (2022), 3, 7198-7211.

[2] Q. Tai et al., Energy Environ. Sci. (2019) 12, 2375.

# NiO<sub>x</sub> nanoparticle including in hole transport layer of inverted p-i-n perovskite solar cell for improvement of its stability

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Since 2009, power conversion efficiency (PCE) of perovskite solar cell has been enhanced from 3.8% to 25.7%. Inverted p-i-n perovskite solar cell is intriguing owing to better compatibility to high throughput manufacturing. It has been reported that hole-transporting self-assembled monolayer (SAM) in p-i-n perovskite solar cell leads to PCE up to 17.8% [1]. Triazatruxene-based hole collecting monolayer (PATAT) in inverted perovskite solar cell further results in PCE up to 23% [2]. Several inorganic hole transport layers (HTL) have been investigated to improve stability. Among HTLs, nickel oxide nanoparticle (NiO<sub>x</sub> NPs) has attracted attention owing to inorganic nature making it stable [3]. Physical properties of NiO<sub>x</sub> NPs have been consequently investigated to improve stability of inverted perovskite solar cells. Inverted perovskite solar cells were fabricated with structure of Glass/ITO/HTL/perovskite absorber/ethylenediammonium diiodide (EDAI<sub>2</sub>)/C<sub>60</sub>/bathocuproine (BCP)/Ag. HTL structures were examined, which are (1) PATAT as reference, (2) NiO<sub>x</sub> NPs HTL, and

(3) NiO<sub>x</sub>NPs/PATAT HTL. NiO<sub>x</sub> NPs synthesis and cell fabrication are discussed elsewhere [2,3]. Stability tests were conducted under 85 °C, dark, and open circuit, as well as maximum power point tracking (MPPT) under 1 SUN. For stability test under 85 °C, performances were periodically evaluated under 1 SUN or 200 lx (LED 5,000 K). PCEs of the p-i-n solar cells are 19% for (1) PATAT, 14.3% for (2) NiO<sub>x</sub> NPs HTL, and 19.3% for (3) NiO<sub>x</sub>NPs/PATAT HTL. PATAT in (3) NiO<sub>x</sub>NPs/PATAT HTL plays a role in enhancing PCE of the solar cells because of passivation of interface defect of NiO<sub>x</sub> NPs. For stability test under 85 °C, ratios of PCE at final hour of 426 hours to that at initial hour (PCE<sub>426h</sub>/PCE<sub>0h</sub>) are 0.71 for (1) PATAT, 0.54 for (2) NiO<sub>x</sub> NPs HTL, and 0.79 for (3) NiO<sub>x</sub>NPs/PATAT HTL under 1 SUN. PCE<sub>426h</sub>/PCE<sub>0h</sub> values are 0.19 for (1) PATAT, 0.60 for (2) NiO<sub>x</sub> NPs HTL, and 0.90 for (3) NiO<sub>x</sub>NPs/PATAT HTL under 200 lx. It is implied that (3) NiO<sub>x</sub>NPs/PATAT HTL demonstrates most stability under 1 SUN, as well as both (2) NiO<sub>x</sub> NPs HTL and (3) NiO<sub>x</sub>NPs/PATAT HTL present significantly more stable under 200 lx. Under MPPT, HTL including NiO<sub>x</sub> NPs shows more stable with over 90% of initial PCE after 645 hours. It is considered that inorganic NiO<sub>x</sub> NPs could slow down the failure of the device. The results have proved that NiO<sub>x</sub> NPs can improve the stability of the p-i-n perovskite solar cells.

**Acknowledgement:** This paper is based on results obtained from a project, JPNP21016, subsidized by the New Energy and Industrial Technology Development Organization (NEDO).

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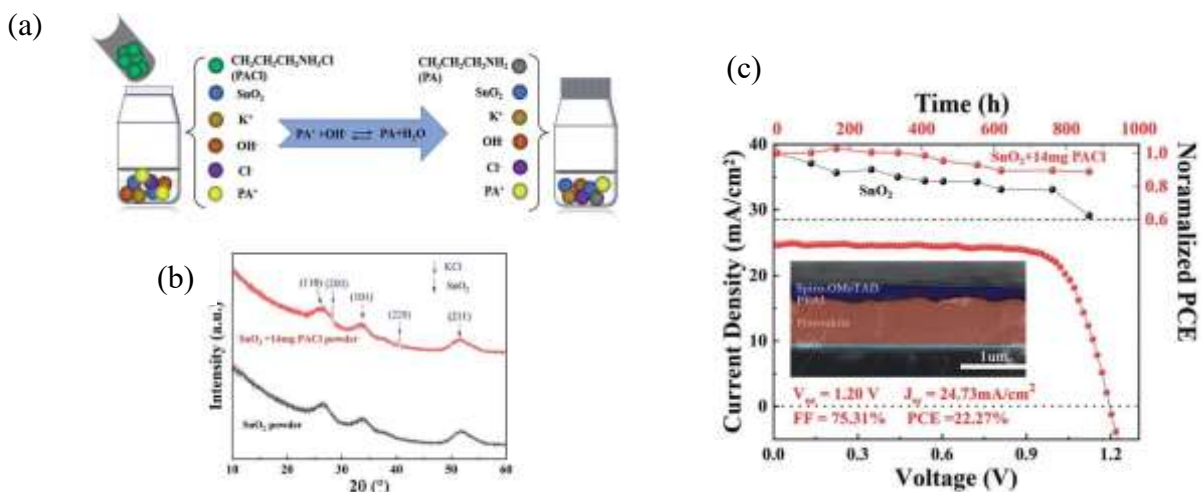
# Organic chloride salt incorporated SnO<sub>2</sub> electron transport layers for improving the performance of perovskite solar cells

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The electron transport layer (ETL) is an integral part of perovskite solar cells (PSCs) to realize efficient carrier extraction and affect the growth of the upper perovskite layer in the n-i-p configuration<sup>[1,2]</sup>. Adding substances is a common modification or engineering strategy to improve the quality of the solution processed SnO<sub>2</sub> ETLs<sup>[3,4]</sup>. Herein, a modification strategy of SnO<sub>2</sub> ETLs by incorporating an organic ammonium chloride salt, propylammonium chloride (PACl), into the commercial SnO<sub>2</sub> colloidal solution is presented. With the incorporation of PACl, KCl is found to be generated in the alkaline solution of SnO<sub>2</sub> colloidal containing potassium ions. Then the generated KCl and the residual PACl together play a role in improving the optoelectronic characteristics of the SnO<sub>2</sub> films, passivating the interface defects between the ETL and perovskite layer, and enhancing the crystallization of the perovskite films. As a result, the over-all performance of the devices based on SnO<sub>2</sub>-PACl ETLs is remarkably improved. A power conversion efficiency (PCE) of up to 22.27% is achieved in the n-i-p planar PSCs based on the PACl incorporated SnO<sub>2</sub> ETLs. In addition to PACl, the addition of primary alkylammonium chloride with different alkylchains (C<sub>n</sub>H<sub>2n+1</sub>NH<sub>4</sub>Cl, n=1, 2, and 4) to the SnO<sub>2</sub> ETLs is demonstrated to have a similar effect on the PSCs. This work provides a reference for modification of the commercial SnO<sub>2</sub> colloidal solution as well an understanding of the underlying mechanisms.



**Fig. 1** (a) Schematic diagram showing the reaction between PACl and SnO<sub>2</sub> colloidal solution. (b) XRD patterns of the SnO<sub>2</sub> samples with/without PACl. (c) The light J-V curve of the champion device based on SnO<sub>2</sub>-14PACl and the stability of the devices.

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# Functional Multicomponent Nanocrystal Superlattices Comprising Lead Halide Perovskite Nanocrystals

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Cesium lead halide perovskite nanocrystals (NCs), owing to their outstanding optoelectronic properties (high oscillator strength of bright triplet excitons, slow dephasing, minimal inhomogeneous broadening of emission lines), are promising materials for creating coherent macroscopic states that can be utilized in quantum applications. Perovskite NCs self-assembled into ordered superlattices (SLs) with simple cubic packing of cubic NCs have been shown to emit ultrafast (*ca.* 20 ps) superfluorescent light [1]. Further advancement in the field, required for programmable tuning of the collective emission and for building a theoretical framework, relies on the higher-level, exquisite structural engineering of the perovskite NC structures, wherein the use of additional building blocks may allow control over the mutual arrangement and orientation of perovskite nanocubes. We present a wide structural diversity in multicomponent, long-range ordered SLs obtained by shape-directed co-assembly of cubic CsPbBr<sub>3</sub> NCs with the spherical, truncated cuboid and disk-shaped NCs [2,3,4]. When combined with larger spherical NCs, SLs of five structure types form, namely, NaCl-, AlB<sub>2</sub>-, and novel, uncommon to all-sphere assemblies AB<sub>2</sub>- as well as quasi-ternary ABO<sub>3</sub>- and ABO<sub>6</sub>-types with cubes occupying B- and O-sites. Targeted incorporation of truncated cuboid PbS NCs on B-sites results in the formation of ternary ABO<sub>3</sub>-type SLs. Combining perovskite nanocubes with other shape-anisotropic building blocks, such as disk-shaped LaF<sub>3</sub> and NaGdF<sub>4</sub> and truncated cuboid PbS NCs, extends the library of accessible SL structures. Perovskite nanocubes exhibit a high degree of orientational ordering in the SLs. We then demonstrate the effect of the SL structure on the collective optical properties.

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# Defect Passivation Effects in 2-D Halide Perovskite Field-Effect Transistor by Lewis-base Molecules.

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Metal halide perovskites (MHPs) are receiving significant attention for their electronic and optoelectronic properties, but their use in device applications is hindered by issues with lead toxicity and stability. To address these concerns, researchers are exploring tin-based lead-free perovskite materials like  $\text{PEA}_2\text{SnI}_4$ <sup>[1]</sup>, which show promise as p-type field effect transistors due to their intrinsic p-doping nature and improved stability compared to three-dimensional counterparts<sup>[2]</sup>. However, the material faces challenges such as self-oxidation and ion migration along grain boundaries. To overcome these hurdles, we are utilizing Lewis acid-base small molecules to study the defect passivation mechanisms of tin-based perovskites and enhance FET properties. This research could lead to the development of advanced electronic devices based on halide-perovskite materials with improved performance.

## Acknowledgement

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# Investigation of Time and Location Dependent Variations in Electroluminescence Images of Perovskite Solar Cells

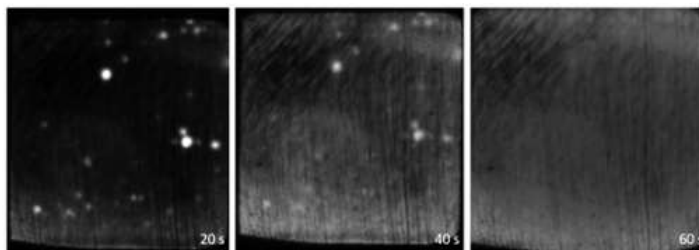
Ennio Luigi Comi<sup>1</sup>

Sandra Jenatsch,<sup>2</sup> Balthasar Blülle<sup>2</sup>, Mattia Battaglia,<sup>1</sup> Christoph Kirsch,<sup>1</sup> Roman Hiestand,<sup>2</sup> Beat Ruhstaller,<sup>1,2</sup> and Evelyne Knapp<sup>1</sup>

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Electroluminescence (EL) imaging [1] of perovskite solar cells (PSC) allows for uniformity analysis of the active layers and the detection of performance limiting factors like resistive losses and shunts. EL signals from perovskite solar cells, however, can vary dynamically after voltage turn-on. This transient behavior in the range of seconds is reported to be attributed to mobile ions in the bulk material and is mostly investigated with a spatially averaged signal [2]. When acquiring electroluminescence images as a function of time we found very pronounced turn-on dynamics in the EL signal that, moreover, varied locally. For our 1.4 cm<sup>2</sup> carbon-based hole-transporter-free perovskite solar cells, the overall behavior reported in [2] was thus confirmed, although the averaged signal was preceded by a strong EL-increase in certain regions. To better understand these local and temporal variations, we first modelled the cell stack with our 1D drift-diffusion simulation software Setfos 5.3, by fitting the material parameters to steady-state and impedance data, and calculated the transient EL signal of a small cell. Through parameter variation, it was found that an increase in the local ion density could reproduce the stronger EL signal at specific locations. The temporal evolution of this peak is strongly influenced by the mobility of iodine vacancies, which was determined by fitting both the measured EL signal and the electrical impedance data. In a second step, current-voltage-luminance (JVL) curves with fixed ion distributions at specific time steps were simulated using the 1D drift-diffusion model. These were then used as input i.e. 1D coupling law for the 2D+1D FEM model in Laoss [1], [3] to solve for the 2D current maps in the two electrodes and the active layer in between. Therefore, with the help the 2D+1D model, we were able to explain the dynamic EL images of a mesoporous perovskite solar cell by local ion density variations.



**Fig. 1: Measured transient EL images at 1.2 V bias at 20, 40, and 60 s after turn-on.**

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# Optimal Interface Engineering through SAM Energy Alignment and Functionalization

Hannah Contreras

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Open circuit voltage losses (VOC) in the perovskite top cell remain a significant challenge for the commercialization of perovskite tandem solar cells. We show through simulations that common hole transport layers like PTAA and Me-4PACz are energetically mismatched with the perovskite active layer which lowers the quasi-Fermi level splitting and limits VOC, particularly for wide bandgap compositions relevant to tandems ( $E_g \geq 1.7$  eV). We identify the ideal energy offset between the hole extraction and the wide bandgap perovskite layers and modulate the anode work function to this ideal using novel halide self-assembled monolayers (SAMs) as interface modifiers. Mixing these SAMs allows for selective tunability of both wettability and work function. Using a two-step deposition, we have not found a clear correlation between improved alignment of the SAM-modified ITO-perovskite interface and improved VOC in solar cell devices. However, we found that mixing the SAMs into the perovskite precursor solution using a one-step deposition method improves their solar cell performance. This suggests that interfacial chemistry, including SAM functionalization and SAM interactions with perovskite in solution, may supersede energy alignment as the primary factor currently limiting VOC. Understanding their respective roles will enable the development of efficient wide gap perovskite devices for Si-tandem applications.

# Investigation of the band alignment at the interface between 2D/3D halide perovskite films and charge extraction layers

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Halide perovskites have attracted a considerable amount of interest for solar cell applications as many approaches have been explored to enhance the stability of these devices. It has been shown that the device architecture, and most importantly the interfaces, are critical for an enhanced device efficiency and stability [1]. In this regard, adding passivation layers or modifying the electron / hole transport layers (ETL/HTL) became a major strategy to achieve stable high-efficiency devices. One of the promising passivation ways is the formation of a two-dimensional (2D) / three-dimensional (3D) perovskite heterostructure. Creating of a 2D/3D structure has proven to improve the interface between the perovskite ETL/HTL in perovskite solar cells [2,3]. However, direct experimental assessment of the electronic properties at the individual interfaces in this complex layer stack remains a major challenge with limited access to the buried interfaces, which eventually require a dedicated approach of surface sensitive.

Here, we form a 2D perovskite layer by spin coating the spacer cation, 4-fluorophenethylammonium iodide, (4-FPEAI) in solution on top of a 3D triple-cation perovskite. We then investigated the energetics and band alignment of the 2D layer formed on the 3D perovskite using ultraviolet and X-ray photoelectron spectroscopy (UPS/XPS) as well as inverse photoelectron spectroscopy (IPES) for varied thicknesses of 2D layers. Afterwards, we deposited a thin layer of the hole transport material Spiro-TTB, ranging in thickness from 5Å to thick 12Å, on top of the 3D perovskite and the 2D/3D structures and employ successive XPS, UPS and IPES measurements at the various steps. We find that the energy level alignment is critically dependent on the 2D/3D layer underneath the hole transport layer and can switch from favorable and unfavorable depending on the thickness of the 2D/3D layer. This study thus paves the route towards a deeper understanding of the 2D/3D electronic properties and energy alignment for a better optimization of the interfaces, helping to increase both the efficiency and stability of devices.

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# Integrated: experimental and theoretical study on structural and magnetic properties of thin films of double perovskite ruthenates; $\text{Ba}_2\text{DyRuO}_6$ & $\text{Sr}_2\text{DyRuO}_6$

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We have grown the novel double perovskite ruthenates viz.,  $\text{Ba}_2\text{DyRuO}_6$  (BDRO) and  $\text{Sr}_2\text{DyRuO}_6$  (SDRO) on the  $\text{SrTiO}_3$  substrate using pulsed laser deposition technique. X-ray diffraction (XRD) data reveal that BDRO forms into a cubic structure, while SDRO forms into a monoclinic structure, similar to that of bulk form [1,2]. UV Visible measurements for both the samples reveal direct influence of A-site element (Sr/Ba) on their band gaps, i.e., 3.66 eV and 2.59 eV for BDRO and SDRO samples respectively, hence suggesting their insulating nature. We have also carried out the first principle calculations within DFT (GGA+U) using the CASTEP software [3] to gain more insights into the experimental data. Temperature-dependent magnetization measurements suggest the presence of ferromagnetism in BDRO, while paramagnetism for SDRO thin film. Surprisingly, both films show canted anti-ferromagnetism at  $\sim T = 5$  K as revealed in their isothermal magnetization curves. The existence of the canted magnetism at a lower temperature may be attributed to the Dzyaloshinskii-Moriya (D- M) interactions [4] in the monoclinic SDRO sample due to structural distortion. Overall, a comparison made between the magnetic properties of both the thin films i.e., BDRO & SDRO reveals the suppression of bulk magnetic ordering when compared to their bulk counterparts. The possible reason for the absence of any magnetic ordering in these thin films may be due to any modifications in super-exchange interactions, any exchange bias, stress-strain, or uncompensated spins present at their interfaces, etc. These thin films with insulating antiferromagnetic properties may be crucial for “Spintronics devices”

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# Engineering polycrystalline Ruddlesden Popper perovskite to achieve wavelength dependent photodetector

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In this work a hot cast BA<sub>2</sub>PbI<sub>4</sub> Metal-Semiconductor-Metal (MSM) photodetector was fabricated and thoroughly investigated. With substrate temperature and deposition speed, the crystal growth of polycrystalline BA<sub>2</sub>PbI<sub>4</sub> was engineered so that closed-packed pinhole-free crystal grains as large as 30×30 μm<sup>2</sup>, that made fast photoresponse of rise and fall time of 187 and 280 μs possible, were achieved. The molarity of Perovskite (PVK) solution controlled the thin film thickness more than morphology. Interestingly, the device characterization showed a wideband photodetector (PD) responding uniformly to wavelengths from 520 to 400 nm fabricated with 0.17 molar PVK solution. However, the 0.46-molar photodetector was way more sensitive to blue light achieving high-responsivity of 119 mA/W under the 450 nm illumination. Where the responsivity of the 0.17-molar PD under 400, 450, and 520 nm illumination was 28, 19, and 23 mA/W respectively, it was 54, 119, and 27 mA/W for 0.46-molar PD. Similarly, the detectivity of the 0.17-molar PD was 2.61×10<sup>7</sup>, 1.8×10<sup>7</sup>, and 2.17×10<sup>7</sup> jones respectively, whereas in the case of 0.46-molar PD it was 1.11×10<sup>8</sup>, 2.15×10<sup>8</sup>, and 5.62×10<sup>7</sup> jones respectively. The standard deviation of the 0.17-molar PD responsivity in different wavelength was 13 percent, but it was 71 percent for 0.46-molar PD the reason was wavelength dependence of light penetration depth in this semiconductor as well as distribution of electric field in PVK layer. These findings were utilized to realize a surface acoustic wave (SAW) UV sensor with sensitivity of 3007.5 ppm/(mW/cm<sup>2</sup>). Here the fabrication and characterization of hot cast BA<sub>2</sub>PbI<sub>4</sub> MSM PD and SAW was reported that for the first time showing outstanding improvement in response time of polycrystalline 2d perovskite via crystal size engineering reducing it to almost 0.01 of similar devices and only comparable with single crystal devices [1, 2], providing responsivity 10 times higher than spin coated devices in 0.46-molar PD [2], and enabling wideband application in 0.17-molar PD.

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# Visualizing Macroscopic Inhomogeneities in Perovskite Solar Cells

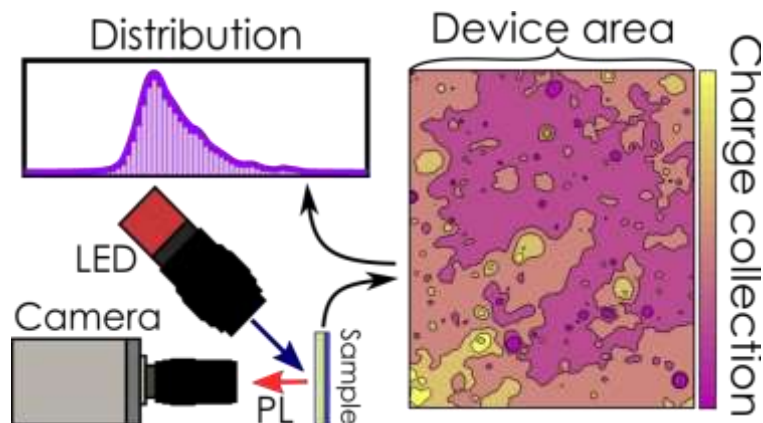
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Despite the incredible progress made, the highest efficiency perovskite solar cells are still restricted to small areas (<1 cm<sup>2</sup>). In large part, this stems from a poor understanding of the widespread spatial heterogeneity in devices. Conventional techniques to assess heterogeneities can be time consuming, operate only at microscopic length scales, and demand specialized equipment. We overcome these limitations by using luminescence imaging to reveal large, millimeter-scale heterogeneities in the inferred electronic properties. We determine spatially resolved maps of “charge collection quality”, measured using the ratio of photoluminescence intensity at open and short circuit. We apply these methods to quantify the inhomogeneities introduced by a wide range of transport layers, thereby ranking them by suitability for upscaling. We reveal that top-contacting transport layers are the dominant source of heterogeneity in the multilayer material stack. We suggest that this methodology can be used to accelerate the development of highly efficient, large-area modules, especially through high-throughput experimentation.



# Advanced study of carrier transport in lead-free double perovskite materials

Elke Debroye<sup>2</sup>

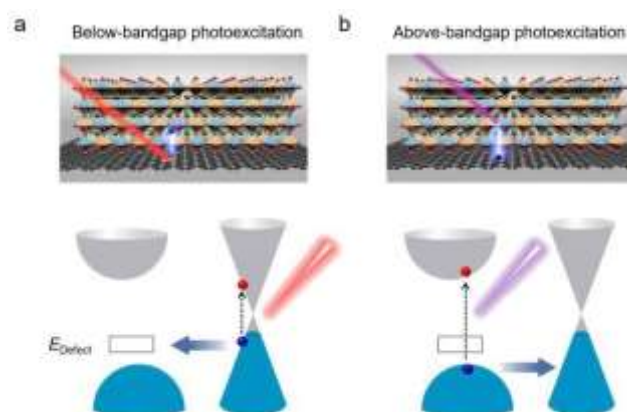
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Cs<sub>2</sub>AgBiBr<sub>6</sub> double perovskite (DP) has emerged as a promising alternative to toxic, unstable lead halide perovskites for various optoelectronic applications owing to its superior chemical stability, nontoxicity, and outstanding photophysical properties. In particular, Cs<sub>2</sub>AgBiBr<sub>6</sub> double perovskite has shown exceptional performance for high-energy photodetection applications. For instance, it exhibits excellent X-ray detection with a low detection limit.<sup>[1,2,3]</sup> Therefore, a study of hot carrier transport in Cs<sub>2</sub>AgBiBr<sub>6</sub> DP following high-energy photoexcitation is of great fundamental interest and could provide insights into their further optoelectronic applications.

I will focus on how we apply a set of advanced spectroscopic tools, including THz spectroscopy, to detail the transport of photogenerated (hot) carriers that govern the optoelectronic performance. We demonstrated a fourfold enhanced hot carrier mobility in Cs<sub>2</sub>AgBiBr<sub>6</sub> DP compared to cold carriers, and a long-range hot carrier transport length beyond 200 nm.<sup>[4]</sup> These findings render Cs<sub>2</sub>AgBiBr<sub>6</sub> as a fascinating platform for hot carrier-based optoelectronic devices. Furthermore, I will discuss the possibility of manipulating the carrier transfer direction and efficiency in DP/graphene heterojunctions (Fig. 1) as new material platform for next-generation optoelectronics.<sup>[5]</sup>



**Figure 1 . Optically controlled hole transfer in a DP/Gr heterostructure in both real (up) and momentum (bottom) spaces for excitation below (a) and above (b) the DP E<sub>bg</sub>.**

[1] W. Pan, et al. *Nature Photonics* (2017), 11, 726–732.

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[3] M. Keshavarz, E. Debroye\*, et al. *Advanced Materials* (2020), 32, 2001878.

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# Visualizing buried interfaces in solution-processed perovskites

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In recent years, metal-halide perovskites have emerged as promising contenders for a wide variety of applications in the field of photovoltaics due to their excellent optoelectronic properties. While these properties can be tuned over a broad range by changing the composition of the perovskite layer, the microstructure of these polycrystalline layers plays a key role in determining their performance and stability. The visualization of the perovskite microstructure is often limited to that obtained by imaging the top surface of layer by techniques such as scanning electron or atomic force microscopy, while buried interfaces are significantly less frequently examined.

In this work, we visualize the microstructure at buried interfaces of triple cation perovskite layer and examine how it is impacted by varying the sample processing conditions. We also examine the development of microstructural flaws at buried interfaces upon degradation. These results are important not only for deposition process optimization, but also for the development of mitigation strategies to suppress degradation at buried interface in perovskite optoelectronic devices.

# Cation passivation and 2D/3D heterostructure: strategies toward high efficient and stable perovskite solar cells

Matteo Degani<sup>1</sup>

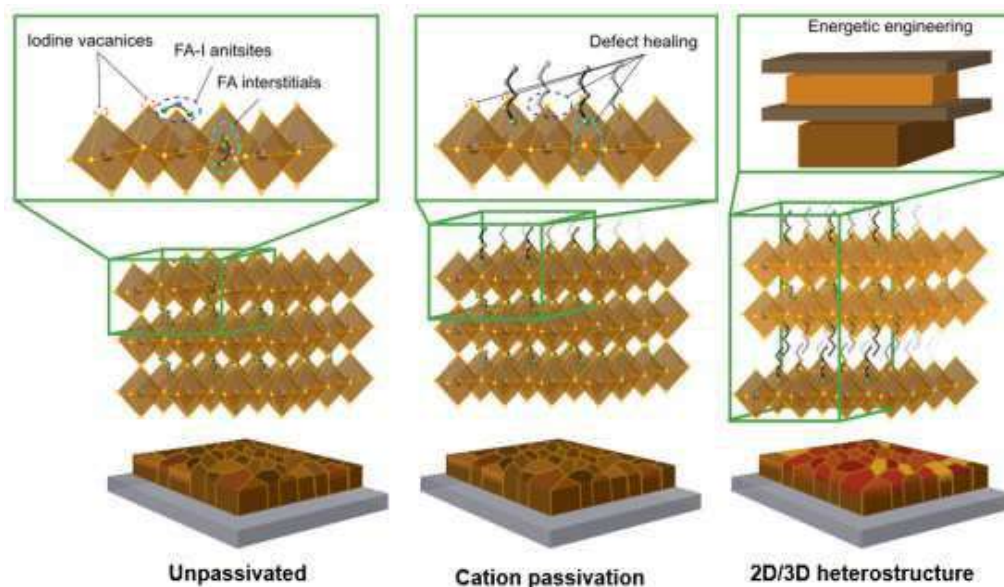
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Three-dimensional (3D)/low-dimensional (LD) perovskite solar cells (PSCs) is one of the leading strategies for the most efficient and stable perovskite solar cells. Despite being one of the most popular and effective way processing techniques, whether the presence of this surface LDP layer - or not- remains elusive. The use of the organic salts without the formation of a LDP, casts the doubts on the effective need for of having this capping layer. In this talk I will compare recent results obtained in the 3D/LDP configuration with the surface cation passivation strategy and 3D/LDP bilayers which both can still produce the highest values perovskite solar cells. I will providing a comprehensive perspective on the benefits from of the two different strategies, showing examples of both strategies with more than 23% efficiency for pin structure<sup>[1]</sup> and for nip structure<sup>[2]</sup>.



**Figure 1** Schematic illustration of defects in perovskite and the two methods described to mitigate them: cation passivation and the 2D/3D heterostructure.

[1] Degani et al, Sci Advances 7, 49, 2021

[2] Degani et al, submitted

# Suppressed Ionic Migration Effects in Mixed Lead-Tin Halide Perovskite Semiconducting Devices

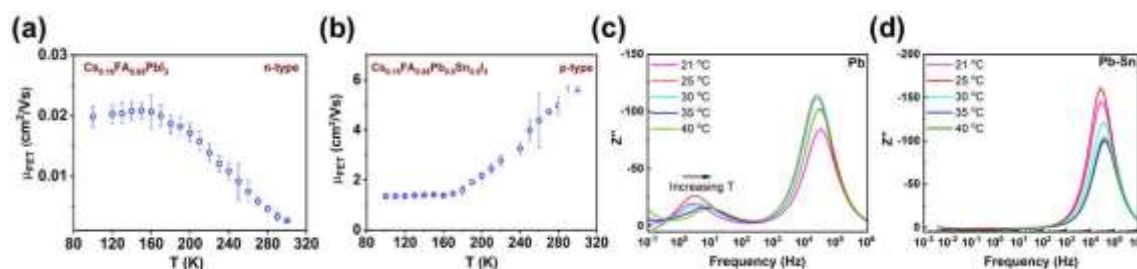
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Despite the meteoric rise in the development of a variety of lead halide perovskite electronic and optoelectronic devices, the phenomenon of ion migration remains a common and longstanding Achilles' heel limiting their performance and operational stability [1,2]. In this talk, I will share our research on understanding the ionic transport in methylammonium-free mixed lead-tin (Pb-Sn) perovskites using two different platforms of perovskite field effect transistors (PeFETs) and perovskite solar cells (PSCs) as platforms, which have thrown up several exciting and heretofore unreported observations that can have important implications for future device development. Firstly, we demonstrate that low bandgap mixed Pb-Sn (Pb:Sn = 1:1) based PeFETs do not suffer from ion migration effects as significantly as their pure-Pb counterparts, thereby reliably exhibiting hysteresis-free p-type transport with high mobility reaching -----5.4 cm<sup>2</sup>/Vs, which is the highest reported value for such compositions [3]. The reduced ion migration is visualized through photoluminescence microscopy under bias and is manifested as an activated temperature dependence of the field-effect mobility (**Fig. 1a-b**) with a low activation energy (~48 meV) consistent with the presence of the shallow defects (such as Sn vacancies etc.) present in these materials. Next, we performed scan- rate dependent current-voltage (and hysteresis) measurements and temperature dependent impedance spectroscopy measurements (**Fig. 1c-d**) on optimized MA-free Pb and Pb-Sn perovskite solar cells, which demonstrate the suppressed motion of ions in Pb-Sn devices as compared to their Pb-only analogues [4], thereby generalizing our earlier observations from PeFETs. We also obtain mechanistic insights into these experimental observations by conducting first-principles calculations. All in all, our results emphasize the relatively unexplored bright prospect of tin substitution in arresting undesirable ionic migration effects in Pb halide perovskite devices.



**Fig. 1:** (a-b) Temperature dependent field effect mobility of optimized Pb and Pb-Sn perovskite FETs. (c-d) Plots of the imaginary impedance against frequency (from impedance spectroscopy) for the corresponding Pb and Pb-Sn perovskite solar cells within a range of temperatures (21 – 40 oC).

[1] K. Sakhatskyi *et al.*, *ACS Energy Lett.* (2022), 7, 3401-3414.

[2] F. Paulus, C. Tzynik, O. D. Jurchescu and Y. Vaynzof, *Adv. Func. Mater.* (2021), 31, 2101029. [3] S. P. Senanayak\* and K. Dey\* *et al.*, *Nature Materials* (2023), 22, 216-224.

[4] K. Dey *et al.*, submitted.

# Investigating the viability of solution processed metal oxides as the hole-extracting layer in tin perovskite photovoltaics

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Tin (Sn) perovskite photovoltaics (PPVs) offer a promising approach to reduce the toxicity concerns associated with lead (Pb)-based PPVs [1]. However, the poor stability of Sn PPVs remains a major barrier to their development. The most widely used hole extraction layer in Sn PPVs is poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), which offers high transparency in the visible light region, high electrical conductivity and high work function [2]. However, PEDOT:PSS is hygroscopic and acidic and is believed to be a source of instability in Sn-PPVs [3]. This poster will present the promising results of a study looking at replacing the PEDOT:PSS hole-extracting layer in Sn PPVs with a solution processed layer of metal oxide.

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[1] M. Ren, X. Qian, Y. Chen, T. Wang, and Y. Zhao, *J Hazard Mater* (2022), 426, 127848.

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[3] Y. Xia, G. Yan, and J. Lin, *Nanomaterials* (2021), 11, 3119.



# Photophysics of Tin-Lead Halide Perovskites for Tandem Photovoltaics

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Due to the outstanding optoelectronic properties and wide applications of organic-inorganic metal halide perovskites, they have attracted enormous attention throughout the photovoltaic community. Perovskite solar cells (PSCs) using lead (Pb) halide perovskites can now reach over 25% power conversion efficiency (PCE), retaining over 90% of their original PCE after 500 hours of light exposure.<sup>1</sup> However, the energy bandgaps of Pb halide perovskites are larger than the ideal bandgap for single junction solar cells, according to the Shockley-Queisser (SQ) radiative limit. Mixed tin-lead (Sn-Pb) halide perovskites will play a pivotal role in approaching the SQ limit where their bandgap can be tuned to below 1.2 eV, which is promising to fabricate highly efficient all-perovskite tandem solar cells. In this work, we report the photophysics behind using guanidium thiocyanate (GaSCN) as an additive to improve the mixed Sn-Pb halide perovskite thin film quality and the resulting device performance. We discuss trends in steady-state and time-resolved photoluminescence spectroscopy and compare the quantum yields of the polycrystalline films. This provides new design rules to understand GASCN additives in low-bandgap Sn-Pb halide perovskite thin films and devices, promoting further research into various approaches to obtain efficient tandem solar cells.

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[1] Min, H., Lee, D.Y., Kim, J. et al. Perovskite solar cells with atomically coherent interlayers on SnO<sub>2</sub> electrodes. *Nature* 598, 444–450 (2021).

[2] Kim, H., Lee, J. W., Han, G. R., Kim, Y. J., Kim, S. H., Kim, S. K., Kwak, S. K., Oh, J. H., Highly Efficient Hole Transport Layer-Free Low Bandgap Mixed Pb–Sn Perovskite Solar Cells Enabled by a Binary Additive System. *Adv. Funct. Mater.* 2022, 32, 2110069.

[3] Feng Lv, Yanqing Yao, Cunyun ke xu, Dingyu Liu, Liping Liao, Gang Wang, Guangdong Zhou, Xusheng Zhao, Debei Liu, Xiude Yang, and Qunliang Song *ACS Applied Energy Materials* 2021 4 (2), 1294-1301

# Structure and properties investigations of carbazole-based monolayers with different functional groups for perovskite solar cells

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Self-assembled monolayers (SAMs) are becoming the reference for hole-transporting materials in inverted perovskite solar cells (iPSCs) due to easy layer formation and low material cost. One of the most well-known SAMs is phosphonic acid with a carbazole moiety and various functional groups [1]. Although SAMs have shown promising results, there is still a lack of information on how the molecular structure of the SAMs is related to the electrical properties of the iPSC. While SAMs are also used in other photovoltaic devices such as organic solar cells, perovskite/Si or perovskite/CIGS tandems [2], understanding how structural changes in SAMs molecules are linked to their electrical properties in photovoltaic devices is crucial for creating molecules with optimal performance and efficiency in each device.

The ability of certain anchoring groups, such as phosphonic acid, to form a monolayer with strong bonds with the surface of the oxides is well established in the literature. [3]. However, little is known about how the position of the functional groups in the chromophore affects the properties (such as wetting angle, surface passivation, work function fine-tuning) of the monolayers and the efficiency of the device.

In this work, a series of molecules with phenyl functional groups were synthesized and tested as hole-transporting materials in iPSC devices. The results indicated that the position of the phenyl substituent has a significant impact on the device efficiency. Specifically, phenyl substituents located at the 3 and 6 positions of carbazole moiety exhibited a similar efficiency as known SAMs molecule (Me-4PACz) [1], while substituents at the 4 positions led to lower efficiency. These findings demonstrate the possible importance of careful molecular design and optimization in developing efficient hole-transporting materials for photovoltaic devices. Further synthesis of molecules with different functional groups and analysis of the abilities are being performed in order to gain a better understanding of the relationship between the functional group placement on the carbazole moiety and photovoltaic device performance.

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[1] A. Al-Ashouri et al, *Science* (2020), 370, 1300–1309

[2] M. Jošt. et al., *ACS Energy Letters* (2022), 7, 1298–1307

[3] S.A. Paniagua et al., *Chemical Reviews* (2016), 116, 7117–7158

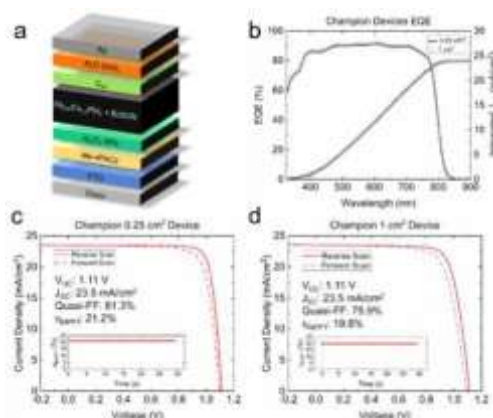
# Factors Affecting Combined Thermal and Light Stability of Inverted Architecture Formamidinium-Cesium Lead Triiodide Perovskite Solar Cells

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While FAPbI<sub>3</sub> and MAPbI<sub>3</sub> perovskite materials are promising candidates for high- efficiency photovoltaic applications, they are ultimately hampered by a lack of thermal and photostability [1]. Mixed formamidinium-cesium lead triiodide (FA<sub>1-x</sub>Cs<sub>x</sub>PbI<sub>3</sub>) materials are shown to improve these properties [2]. In this work, we take a novel approach to the optimization of FA<sub>1-x</sub>Cs<sub>x</sub>PbI<sub>3</sub> perovskite devices by using one of the most challenging ISOS stability protocols of combined elevated temperature and continuous light soaking at open circuit (ISOS-L-2) as a benchmark during every step of the process [3]. We introduce a benzylammonium thiocyanate bulk additive, improve inverted architecture top contacts, and examine the effect of PbI<sub>2</sub> composition to increase 1.55 eV FA<sub>0.8</sub>Cs<sub>0.2</sub>PbI<sub>3</sub> perovskite device stability under the ISOS-L-2 protocol. We find benzylammonium thiocyanate yields improved device stability and maximum power point tracked efficiency as high as 21.2%. Adding a sputtered transparent conducting oxide interlayer top contact as a barrier on top of ALD SnO<sub>2</sub> before the top metal electrode is demonstrated to further boost device stability. PbI<sub>2</sub> excess in the perovskite precursor stoichiometry is shown to have a positive effect on device stability when combined with EDAI<sub>2</sub> surface treatment. These results enable us to better understand relevant factors that affect the stability of inverted FA<sub>0.8</sub>Cs<sub>0.2</sub>PbI<sub>3</sub> perovskite devices with efficiencies over 20% under real-world conditions.



**Figure 1.** a) p-i-n inverted architecture for 1.55 eV champion devices: FTO/Me-4PACz/Al<sub>2</sub>O<sub>3</sub> nanoparticles/FA<sub>0.8</sub>Cs<sub>0.2</sub>PbI<sub>3</sub> + 0.2 mol% benzylammonium thiocyanate bulk additive/7 mM EDAI<sub>2</sub> surface treatment/25 nm C60/20 nm ALD SnO<sub>2</sub>/100 nm Sputter IZO/100 nm Au. b) External quantum efficiency spectrum and integrated JSC of champion 0.25 & 1 cm<sup>2</sup> area devices shown in Figures 1c & 1d. c) JV-curve of champion 0.25 cm<sup>2</sup> area device displayed in Figure 1a. Stabilized open-circuit voltage (V<sub>oc</sub>), stabilized short-circuit current (J<sub>sc</sub>), maximum power point tracked efficiency (□MPPT), and quasi-fill factor are included. □MPPT measured over 30 seconds is also graphed. d) Same characteristics for champion 1 cm<sup>2</sup> area device.

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# **In-situ characterization of metal halide perovskite formation from environmentally friendly solvents using in situ wide and small angle X-ray scattering**

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Interest in wet chemical synthesis to produce metal halide perovskite powder has increased in recent years because it allows for easy production of large quantities of perovskite crystals and when used to produce thin perovskite films for solar cell applications the resulting device exhibit high stability and performance [1,2]. The stoichiometric homogeneity achieved by the crystallisation process in the alcohol dispersions simplifies thin film deposition and therefore improves photovoltaic device performance over large areas. In this study we compare methanol, ethanol, propan-2-ol and pentanol as solvents for precipitation reactions forming methyl ammonium lead iodide MAPbI<sub>3</sub> and methyl ammonium formamidinium lead iodide MA<sub>0.5</sub>FA<sub>0.5</sub>PbI<sub>3</sub> perovskites. Using time resolved in-situ small and wide X-ray scattering (SAXS and WAXS), we were able to follow the reaction of the dissolved methylammonium iodide and formamidinium iodide with the suspended lead iodide determine the mechanism whereby the structural assembly occurs from precursors to perovskite. These measurements led to a deeper understanding of intermediate steps during the reaction, where particle morphology control is possible during the perovskite material assembly. The precipitation method to produce metal halide perovskite described in this work is cost-effective and has less safety issues due to low solvent toxicity. This work outlines an alternative processing route for stable photovoltaics based on perovskite powder.

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[1] M. B. Johansson et al., *Nano Energy*, 78 (2020), M. B. Johansson et al., *ECS, Journal of Solid State Science and Technology*, 5 (2016)

[2] Konstantinos Tsevas et al., *Chemistry of Materials* 2021 33 (2), 554-566 DOI:10.1021/acs.chemmater.0c03517

# Investigating the Interplay between Microstructure and Carrier Dynamics in Two-Dimensional Perovskites

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Quasi-two-dimensional (2D) lead-halide perovskites have gained significant attention in the field of photovoltaics (PV), due to their remarkable optical and photophysical properties and improved stability compared to their 3D counterparts [1]. The quasi-2D perovskites consist of  $n$  blocks of inorganic  $[\text{PbI}_6]^{4-}$  octahedral layers separated by large organic cations. In general, a single film contains multiple perovskite phases characterized by different values of  $n$  ( $n=1,2,3\dots\infty$ ) and distinct bandgaps [2]. Upon excitation, quantum confinement in the low- $n$  phases introduces excitons alongside the free carriers created in the high- $n$  phases [3], causing interesting and complicated carrier dynamics. Despite the significant influence of the crystallization and fabrication parameters on the ultrafast photophysical processes, the relationship between film microstructure and its optoelectronic properties remains poorly understood. To investigate this, we utilized solvent and spacer engineering approaches to fabricate quasi-2D perovskite thin films with various microstructures (Fig. 1). We then probed the ultrafast photophysical processes through time-resolved spectroscopy techniques, such as time-resolved photoluminescence (TRPL) and ultrafast transient absorption (TA). While TRPL only detects emissive processes, TA can also probe non-emissive processes on a femtosecond time scale, such as hot carrier cooling and charge transfer from low- $n$  to high- $n$  phases. This offers unique insights into the design and optimization of quasi-2D perovskite materials for a new generation of PV devices.

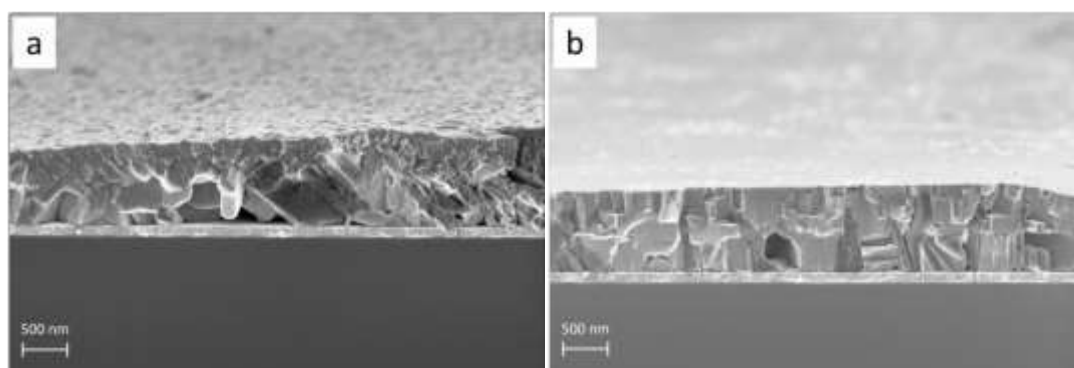


Figure 1: SEM images of randomly oriented (a) and vertically oriented (b) quasi-2D perovskite film

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# Interface and Device Engineering Toward High Performance Flexible Perovskite Solar Cells

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The newly emerging photovoltaic technology based on organo-metal halide perovskite solar cells (PSC) is a competing contender with the currently dominating silicon solar cells. PSC show promising optoelectronic properties including long carrier lifetimes, high light absorption, low cost and lightweight, reaching a power conversion efficiency (PCE) of 25.7% [1]. Device stability does, however, remain a challenging issues, despite much progress. There are many causes of PSC degradation, but some of the most common triggers are oxygen, moisture, heat, and light. The perovskite layer, as well as the charge transport layers, can decompose or undergo phase transitions, and all the interfaces between those layers are susceptible to undesired changes [2]. Despite these challenges, the low temperature processing of perovskite film makes it uniquely suitable for flexible PSC (*f*-PSC) owing to characteristic low formation energies. Which is desirable but restrict the high mechanical endurance due to low toughness originating from low temperature processability of polycrystalline perovskite film [3-5]. Further, the presence of toxic lead-containing compounds in the perovskite film, posing a potential threat to the environment. To tackle these challenges, *f*-PSC is demonstrated using an interlayer between perovskite and electron transporting layers with the objectives to achieve high stability and efficiency, utilize external strain via the piezo-phototronic effect, capability to adsorb the toxic lead along with high mechanical endurance.

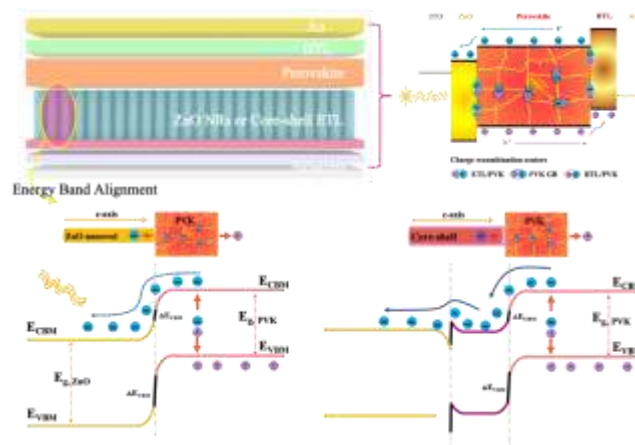


Figure 1. Device structure and charge transport mechanism at ETL/perovskite interface using nanorods or core-shell ETL.

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[2]Rong, Y., Hu, Y., Mei, A. *et al.* Science (2018), 361, 6408.  
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# Probing and quantifying Förster-like energy transfer from single perovskite quantum dots to organic dyes

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A vast parameter space emerges upon coupling quantum dots (QDs) with organic molecules in hybrid nanoassemblies, entailing a manifold of new properties and applications. For instance, employing hybrid assemblies in photocatalytic reactions could significantly exceed the performance of the individual constituents exploiting the very large absorption cross section of QDs in combination with the long-lived excited states in organic molecules [1,2]. However, understanding the complex behaviour arising in hybrid nanoassemblies requires methods with high spatio-temporal resolution hindering the rational design of functional nanomaterials [3]. Here, we probe energy transfer (ET) from single lead halide perovskite QDs to organic dye molecules employing single-particle photoluminescence spectroscopy with single-photon resolution. We identify ET by spatial, temporal, and photon-photon correlations in the QD and dye emission. Exploiting the high temporal resolution of our experiment as well as the discrete quenching steps due to photobleaching of individual organic dyes, we observe a characteristic Förster-type ET, with efficiencies higher than 70% in the sole case of a strong donor-acceptor spectral overlap. Our work sheds light on the processes occurring at the QD/molecule interface and demonstrates the feasibility of performing photocatalytic reactions exploiting efficient ET from QDs to organic catalysts.

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# Electrostatically triggered autonomous self-healable and stretchable hydrogel for flexible perovskite solar cells

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The expeditious growth of self-healable multifunctional electronics poses a challenge on power devices to acquire fast autonomous self-healing of solids with efficient electrical recovery. However, realizing this goal remains elusive due to the sluggish dynamics of covalent and ionically linked ions. Herein, we overcome this limitation by introducing electrostatic and hydrogen bonding centers in solids to accelerate ion dynamics via more delocalization centers. As such, the matrix is able to retain fast autonomous self-healing (A-SH) characteristics in dry, wet, and frozen states via an electrostatically driven diffusion-less self-healing mechanism. The self-healable, stretchable, transparent hydrogel after eutrophication to dimethyl sulfoxide is utilized as a scaffold in the perovskite crystallization process, thereby passivating the structural defects at grain boundaries and improving charge transport properties [3,4]. This organogel bridged structural design endows excellent mechanical endurance and preserves the morphology after mechanical cycling. Furthermore, the detrimental cracks induced during repeated deformation can be effectively self-healed autonomously within minutes via fast reforming intramolecular/intermolecular hydrogen bonds.

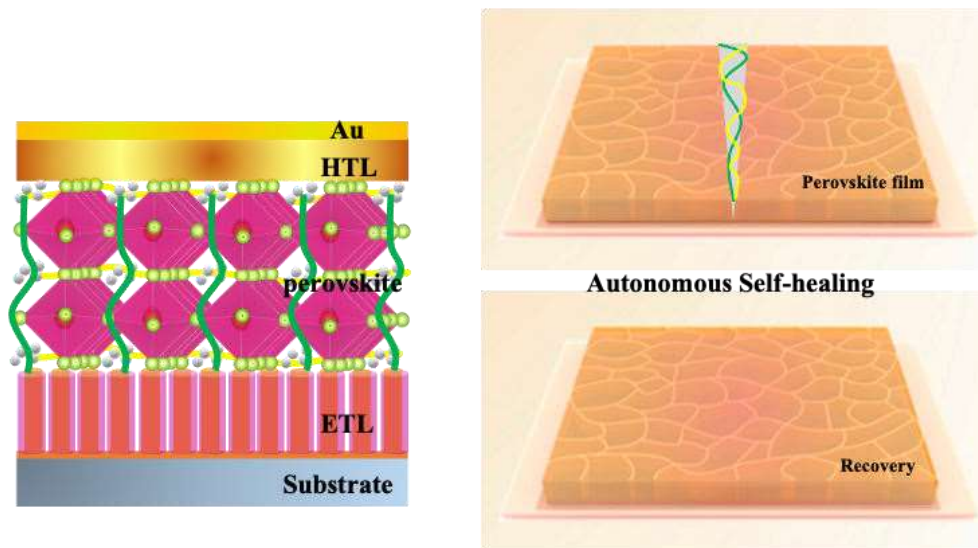


Figure 1. Device structure with perovskite film cross-linked with autonomous self-healable hydrogel.

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# Designing Ytterbium-doped perovskite near-IR emitters: the role of dimensionality and crystal geometry

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As perovskites continue to raise interest for light emitting application, doping with guest atoms has emerged as a promising strategy to achieve monochromatic emission from atomic transitions [1]. Specifically, research has focused on exploiting transitions between d- or f- orbitals in transition metals (e.g. Mg [2]) and lanthanides (Eu, Yb [3,4]) which have successfully been integrated in perovskite matrixes to achieve emission in the visible and NIR range. Ytterbium in particular is a promising dopant for emission in the near IR, as transition between its f-orbitals are emissive in the 1000 nm spectral region. Until now, studies on Yb doped perovskite have focused on CsPbX<sub>3</sub> nanocrystals and quantum dots, where spatial confinement can facilitate recombination on the guest atoms [3,5,6]. In this work we focus on the integration of Yb atoms in perovskite thin films, exploring the effect of not only energy band overlap but also of the materials structural properties. Combining static and time-resolved spectroscopic characterization as well as X-Ray diffraction, we isolate the effect of halide composition, choice of cation and perovskite dimensionality on Yb emission. In particular, we highlight the role of the perovskite crystal field on Yb luminescence, show effective population transfer to dopant atoms in MAPbX(Cl<sub>x</sub>Br<sub>1-x</sub>)<sub>3</sub> and we integrate an Yb-doped MAPbCl<sub>3</sub> thin film in a NIR LED.

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# Transient Electroabsorption Spectroscopy Reveals Direct Tracking and Extraction of Charge Carriers from Hybrid Perovskites

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While perovskite solar cells have achieved power conversion efficiencies exceeding 26%, there still remains a lack of complete understanding of the fundamental processes governing the operation of these devices. In particular, information about charge carrier transport across the perovskite layer to the selective contacts is still very much in dispute. In semiconductors, the motion of charge carriers plays a crucial role and is affected by their mobility and diffusivity. However, in perovskites, the characterization and understanding of charge carrier mobility and diffusivity is still lacking. The mobility values of perovskites vary by many orders of magnitude depending on the material processing conditions, device architecture, and measurement techniques [1]. In most cases, the samples used for mobility evaluations differ from those used in real devices, making the applicability of mobility values questionable [2].

The present study focuses on the investigation of charge carrier motion and extraction dynamics in hybrid perovskite solar cells using the ultrafast electric field modulated transient absorption technique. This technique allows us to directly evaluate the electric field dynamics and visualize the motion of charge carriers with subpicosecond temporal resolution. Our results show that photogenerated holes drift across the mesoporous TiO<sub>2</sub>/perovskite layer during several hundred picoseconds. While hole extraction into the Spiro-OMeTAD layer occurs within tens of nanoseconds, suggesting that hole extraction is limited by the perovskite/Spiro-OMeTAD interface rather than by hole transport through the perovskite layer. In addition, we employ the ultrafast time-resolved fluorescence technique, which shows a fluorescence decay during tens of picoseconds. This decay is attributed to the spatial separation of electrons and holes within the solar cell.

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# Using the Ionic Liquids (ILs) as the Additives to Enhance the Perovskite Solar Devices Stability and Efficiency

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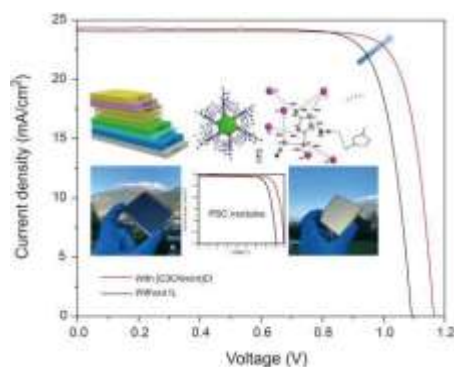
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Perovskite solar cells (PSCs) have been attracting growing attention in the past few years due to the rapid rise in their power conversion efficiencies (PCEs) from 3.8 to 25.8% [1]. As the PCE is approaching the theoretical maximum, the most crucial issue concerns long-term stability which is still a major concern and represents a major bottleneck to commercialization. Several problems are associated with the instability of PSCs, due to the hydrolysis of the perovskites when exposed to moisture.

To overcome these problems, numerous techniques have been developed. Ionic liquids (ILs), being non-volatile salts with high thermal stability, are attractive for a broad range of energy-related applications. ILs have been incorporated into PSCs including the organ- inorganic and all inorganic systems as passivation agents in the perovskite layer resulting in improved device stability and performance.

We have designed and synthesized new functionalized ILs with  $\text{Cl}^-$  and  $[\text{TFSI}]^-$  anion, then a series of PSC devices employing the perovskite films prepared from the IL- precursor solutions were fabricated using n-i-p architecture [2,3]. Up to now, using different ILs as additives will be achieved higher PCE. It is worth highlighting that the long-term stability of perovskite films has also revealed that the introduction of designed ILs is much helpful in enhancing the stability of perovskite solar cells and solar modules.



**Figure 1. IL additives for PSCs result in good PCE for small cells and large modules.**

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# Experimental determination of exciton binding energy, exciton-phonon interaction and Urbach energy in $\gamma$ -CsPbI<sub>3</sub> nanoparticles.

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Cesium lead triiodide (CsPbI<sub>3</sub>) has recently drowned the attention of the perovskite community for its success in the implementation of high-performance optoelectronic devices as solar cells and light emitting devices (LEDs) [1,2]. Orthorhombic  $\gamma$ -CsPbI<sub>3</sub> possesses the highest structural stability among the optically active (light-emissive) CsPbI<sub>3</sub> perovskites. Despite the great interest this material has aroused its fundamental properties have been only barely studied. In this work  $\gamma$ -CsPbI<sub>3</sub> nanoparticles, synthesized by the hot-injection technique, were examined using low-temperature (10K

– 290K) photoluminescence and optical transmission spectroscopy techniques. This enabled the determination of several important parameters for the implementation of optoelectronic devices by studying fundamental quantum processes of absorption and emission near the bandgap [3]. The findings reveal that inorganic perovskites display prominent excitonic behavior, especially evident in low-temperature absorbance spectra. Fitting these spectra with Elliott's model several important fundamental parameters were obtained, such as the excitonic absorption energy and its spectral width, Urbach energy, and bandgap energy, which was then used to determine temperature dependence of the exciton binding energy. Furthermore, by analyzing variations in the photoluminescence spectrum shape with temperature and excitation power it was possible to prove that in  $\gamma$ -CsPbI<sub>3</sub> photoluminescence is originated in excitonic recombination. Besides, it was also possible to prove that the interaction of excitons with phonons occurs mainly through LO phonons, especially at room temperatures. Exciton-phonon interaction is produced by a phononic mode with an effective energy that can be calculated using Segall's model of exciton-phonon interaction. Results show that this characteristic energy is  $15 \pm 1$  meV in  $\gamma$ -CsPbI<sub>3</sub> nanoparticles. In addition, the Arrhenius diagram was used to obtain the energies associated with the mechanisms that produce photoluminescence quenching. This channel, with associated energy of  $27 \pm 2$  meV, corresponds to the thermal dissociation of excitons and is a measurement of exciton binding energy. This value is close to thermal energy what ensures that most excitons will dissociate at room temperature.

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# Evaporation-Solution Deposition of >20% Efficient FAPbI<sub>3</sub>-Based Perovskite Solar Cell as Mid-cell for Triple Junction Solar Cells

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With 32% efficiency achieved for double junction silicon/perovskite tandem, further efficiency improvement will soon be physically limited. To further enhance the efficiency while reducing the leveled cost of electricity, multi-junction devices beyond dual junctions such as triple junctions (especially tandems based on silicon/perovskite/perovskite) are promising candidates. For this purpose, based on optical simulations, we identify FAPbI<sub>3</sub>-based perovskites as an excellent candidate for mid-cell absorber (current matching at 14 mA/cm<sup>2</sup>). Stabilizing FAPbI<sub>3</sub>-based perovskites with high efficiency, however, is a challenging task, which we address in this research. The perovskite films were deposited by the evaporation of PbI<sub>2</sub>:CsBr template films and then spin coating of organohalide solution, followed by annealing of the samples at temperatures as low as 150 °C. The perovskite films contain only minimal traces of PbI<sub>2</sub>, evident from the X-ray diffractograms, pointing towards complete crystallization. We observe large domains around 1000 nm and a surface roughness of 65 nm for a thickness of about 800 nm for an optical bandgap of 1.54 eV. Our simulation indicates that such an absorber inserted in a triple junction with 310 nm thick 1.8 eV top cell material would lead to current of >13.09 mA/cm<sup>2</sup> compared to the ~13.97 mA/cm<sup>2</sup> current in the top cell and 15.05 mA/cm<sup>2</sup> current in the bottom cell (highly top limited region). Perovskite films deposited on indium tin oxide/self-assembled-monolayer (ITO/SAM) stack show a photoluminescence quantum yield of 0.5% leading to a quasi-Fermi level splitting of 1.08±0.02 eV and non-radiative losses of <140±10 meV. Planar devices (ITO/MeO-2PACz/Perovskite/C60/SnOx/Ag configuration) exhibit efficiencies up to 20.73% (JSC >22.98 mA/cm<sup>2</sup>, VOC >1.094 V, FF >82.43%) and stabilized maximum power point output >20%. These results show great potential of FAPbI<sub>3</sub>-based perovskite films for using as a single- and multi-junction devices.

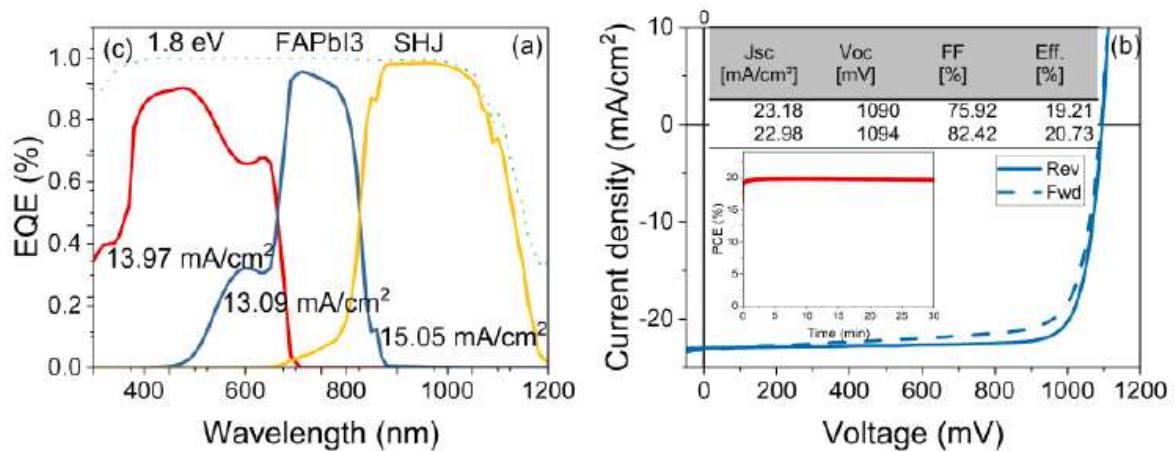


Figure 1. (a) Simulated EQE for triple junction device, (b) J-V curve, J-V characteristics, and MPP tracking of the champion device.

# Treatment of perovskite solar cells by cesium chloride: towards inorganic Ruddlesden-Popper phase passivation for hybrid perovskite

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Metal halide perovskite (MHP) solar cells are currently the fastest growing photovoltaic technology, with new record efficiencies announced regularly. However, these impressive efficiencies come with a severe drawback going forward to the industrialization of the technology, which is device instability under different stresses, notably heat and illumination. Though the mechanisms of this instability are still uncertain, some key elements have been highlighted as drivers for the degradation of the perovskite, especially ionic migration [1] and crystalline defects [2].

Among the strategies for mitigating this degradation, the incorporation of Ruddlesden-Popper (RP) phases, or 2D perovskites, has been largely explored with hybrid 2D phases based on large organic cations. However, fully inorganic Ruddlesden-Popper phases such as  $\text{Cs}_2\text{PbI}_2\text{Cl}_2$  have also displayed promising results for suppression of ion migration and passivation of the grains boundaries when incorporated into inorganic perovskite solar cells by CsCl treatment [3,4]. In this study, we aim at transferring these results to hybrid perovskites. The present work shows the passivating effects of CsCl addition into a hybrid perovskite through different processes, and examines whether the forced formation of the RP phase  $\text{Cs}_2\text{PbI}_2\text{Cl}_2$  is effective and could be beneficial.

Firstly, we show that the addition of CsCl by different processes results in a clear passivation of the perovskite layer, as revealed by photoluminescence (PL) spectroscopy measurements. Indeed, for half-stack (HTL/MHP) measurements, the PL intensity is multiplied by a factor of 2 to 10, clearly signifying a passivation of the defects in the perovskite film. This effect is preserved, although to a smaller degree, for the completed cell, with a  $\text{C}_{60}$  ETL on top of the perovskite: despite the creation of a highly defective interface between MHP and  $\text{C}_{60}$ , which causes a massive collapse of PL intensity for all compositions, the PL intensity of CsCl-treated samples was higher than the reference by a factor of up to 5, meaning that the CsCl passivation also seems beneficial for the quality of the limiting ETL/MHP interface.

These PL results are validated by measurements of the photovoltaic parameters of reference and passivated cells, which reveal that the passivation translates to similar or improved values for  $V_{oc}$ ,  $J_{sc}$  and FF, even yielding in the best case an improved PCE of 17.9% compared to the reference at 17.4%.

At the same time, we present the results of the first advanced characterizations techniques enabling us to interpret the nature of the passivating layer (CsCl or RP phase  $\text{Cs}_2\text{PbI}_2\text{Cl}_2$ ) depending on the CsCl integration process.

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# Interlayer engineering enhances responsivity of perovskite lateral photoconductors for X-ray detection

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Metal halide perovskites are a groundbreaking family of semiconductors finding applications on several areas of the optoelectronics field. They have attracted attention for their bandgap tunability (1.2-3.2eV), long carrier lifetimes, high defect tolerance and solution processable fabrication [1, 2]. Specifically for X-rays detection, their large absorption coefficient allows efficient beam absorption even for low thicknesses, associated with the large-Z elements in their composition (Sn, I, Cs, Pb, Bi). In fact, they have already overcome the state-of-the-art X-ray detectors becoming a serious candidate for the next generation of devices [3].

From the possible architectures, lateral photoconductors excel in their simple and low cost integration with electronic backplanes, facilitating the technology transfer to a viable commercial direct detector. However, lateral photoconductors suffer from lower sensitivity and larger dark current than alternative architectures. To tackle this, fullerenes were incorporated as interlayer (C60) and additive (PC<sub>60</sub>BM) in devices with Au or ITO interdigitated electrodes. We follow an easy and scalable fabrication method that relies on blade coating an ink of MAPbI<sub>3</sub>, yielding a semi-porous film [4].

First, the effect of each fullerene in both Au/MAPbI<sub>3</sub>/Au and ITO/MAPbI<sub>3</sub>/ITO devices was evaluated in terms of dark current suppression and photocurrent enhancement. C60 proved to efficiently decrease the dark current, while PC<sub>60</sub>BM enhanced carrier extraction for all devices, increasing the photocurrent under white light (1 sun). Then, more than the performance, the stability of the performance to ion motion, correlated with the application of a high bias, is investigated. ITO devices proved to be more resilient to poling (500 V/mm) than Au devices, showing stable values of dark and light current over positive and negative poling cycles. Another important observation is the distinction of an “operational dark current” after illumination, different from the dark current for fresh samples. ITO devices showed an improved operational dark current, as opposed to Au devices, which suggests detrimental secondary reactions promoted by light occur in the latter. Finally, a good compromise was achieved in ITO/C60/MAPbI<sub>3</sub>:PC<sub>60</sub>BM/C60/ITO devices, with reduced dark current while enhanced responsivity at 50V/mm, compared to the reference without fullerene. These are the first steps towards history-free, high-sensitive lateral photoconductors for X-ray detection.

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# Achieving Balanced Charge Extraction via Concerted Co-Doping of Charge-Selective Layers for Stable CsPbI<sub>3</sub> Solar Cells

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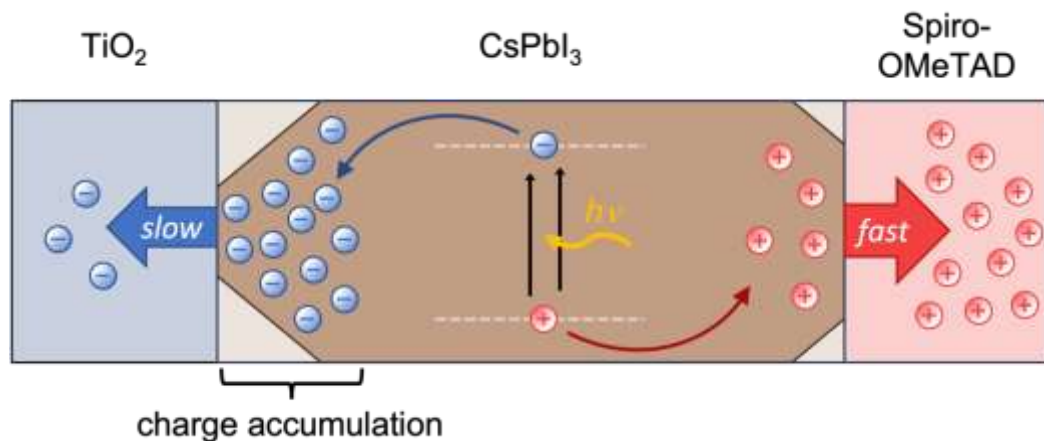
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Solar cells based on inorganic perovskite CsPbI<sub>3</sub> have achieved power-conversion efficiencies (PCEs) of above 20%. Research efforts have mainly focused on the crystallization of the CsPbI<sub>3</sub> perovskite and its passivation. For stable operation, however, it is crucial to thoroughly understand the processes occurring upon charge extraction. In this study, we focus on the charge-selective layers' electronic properties. Based on the model system TiO<sub>2</sub>/CsPbI<sub>3</sub>/spiro-OMeTAD, we modulate the Fermi levels of both charge-selective materials via a co-doping, serving as a lever to fine-tune the energetic alignment with the perovskite. The energetic alignment directly affects the extraction rate across the interface. For the first time, we fully characterize the charge extraction from CsPbI<sub>3</sub> to TiO<sub>2</sub> and spiro-OMeTAD charge-selective layers via transient surface photovoltage. By using Nb(V) and Sn(IV) as inorganic dopants for TiO<sub>2</sub> and spiro- diradical and [TBMP][TFSI] as organic dopants for spiro-OMeTAD, we optimized the charge extraction efficiency, reducing the interface recombination on both interfaces. We show that assembling the optimized CSLs in solar cells does not lead to the best performance, but that the charge extraction across both interfaces show mutual dependence. Furthermore, this study provides a fundamental understanding of interfacial charge extraction that can be transferred to other charge-selective materials.



**Figure 1** Asymmetric charge extraction rates lead to interfacial charge accumulation, triggering degradation pathways in CsPbI<sub>3</sub> perovskite.



# Learning curves from long-term outdoor testing and indoor optoelectronic characterization of perovskite mini-modules

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Improving the performance of perovskite devices is key to increasing their competitiveness against conventional sources of energy. Several perovskite and perovskite on Silicon tandems were extensively investigated both outdoors at real environmental conditions and indoors using a range of advanced optoelectronic methods (Spatially-Resolved Electroluminescence/Photoluminescence, Lock-In-Thermography, Light-Beam Induced Current, Raman and Ultrafast spectroscopy, etc.) to set-up a complete optical and electrical characterization of perovskite devices. The devices demonstrated the impact of irradiance and temperature on their major electrical parameters during outdoor testing conducted over several months in the field. Significant discrepancies on degradation rate were obtained for some perovskite architectures demonstrating the impact of material quality on long-term performance of perovskites. Exponential degradation of performance was obtained in the majority of samples under test during the first hours of light application. Performance recovery overnight and diurnal performance degradation of several perovskite samples were calculated for each day in the field demonstrating the dominant values for diurnal degradation and recovery for each perovskite structure and at different degradation stages. Seasonal dependence of the overall performance degradation is discussed and the diurnal performance degradation-to-recovery ratio is analysed.

Spatially-resolved Electroluminescence and Lock-In-Thermography methods demonstrated hotspot and shunts evolution in perovskite mini-modules after outdoor exposure. Raman spectroscopy measurements revealed the differences in chemical properties of perovskite mini-modules after outdoor exposure while Ultrafast spectroscopy demonstrated the carrier relaxation processes in the devices which are correlated with diurnal performance degradation and recovery processes.

# The effect of solution phase bromide-iodide exchange on the structural and optoelectronic properties of Cs<sub>3</sub>Cu<sub>2</sub>Br<sub>5</sub> layers

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Ternary metal-halide pseudo-perovskites recently gained interest in the field of optoelectronics (e.g., ionizing radiation/light detection, LEDs) because of their unique light emission properties. Cesium copper halides (Cs<sub>3</sub>Cu<sub>2</sub>X<sub>5</sub> and CsCu<sub>2</sub>X<sub>3</sub> where X=Cl, Br and I) are the most prominent members of this materials family. These compounds are considered less toxic and more environmentally stable compared to their metal-halide perovskite predecessors. After excitation the soft lattice (low crystal formation energies) of cesium copper halides allows the formation of self-trapped excitonic states, through lattice distortions. The formed excitons can be trapped at these electronic states within the bandgap, which results in a large Stokes-shift (~ 100 nm for Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub>). This minimizes the reabsorption of light, which property is beneficial for applications that rely on efficient light generation and collection. [1]

Cesium copper halides possess composition tunable optoelectronic properties (e.g., bandgap PL quantum yield, PL peak position and lifetime).[ref] By altering the halide composition the PL lifetime can be fine tuned from 1 μs (Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub>) to 20 μs (Cs<sub>3</sub>Cu<sub>2</sub>Br<sub>5</sub>), with the simultaneous change in the quantum yield. The halide composition can be either altered during synthesis or with post-synthetic approaches (often used in the case of metal-halide perovskites). The halide exchange properties of pseudo-perovskites is not yet fully understood, which would ultimately aid the better design of optoelectronic devices. [2]

In my presentation, the effect of bromide/iodide halide exchange process on the optoelectronic and structural properties of Cs<sub>3</sub>Cu<sub>2</sub>Br<sub>5</sub> thin films will be discussed. To perform the halide exchange 10 μm thick Cs<sub>3</sub>Cu<sub>2</sub>Br<sub>5</sub> layers, prepared by spray coating were immersed into CsI containing methanol solutions. By precisely tuning the immersion conditions (concentration, immersion time) apart from the bulk halide exchange of the layers a phase transition to CsCu<sub>2</sub>I<sub>3</sub> can also be achieved as revealed by X-ray diffraction measurements. SEM revealed that this phase transition also changed the morphology of the layers, as the initial granular structures (Cs<sub>3</sub>Cu<sub>2</sub>X<sub>5</sub>) were gradually changed to rod-like features (CsCu<sub>2</sub>X<sub>3</sub>). The effect of the compositional changes on the PL lifetime, PL maxima as well as the PL quantum yield of the samples will also be discussed.

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# Interface formation between halide perovskites and NiO<sub>x</sub> studied by photoemission spectroscopy

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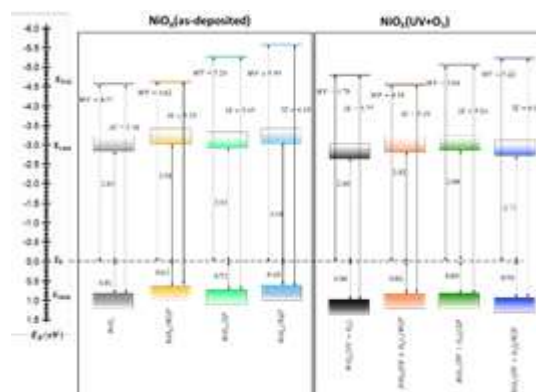
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Metal halide perovskite (MHP) solar cells have revolutionized the field of photovoltaic technologies by achieving a remarkable increase in power conversion efficiency (PCE) from 3.8% to 25.5% [1] within a decade. Challenge remains for researchers to improve the efficiency and stability of MHP-based solar cells towards the theoretical limit of 33% set by Shockley-Queisser<sup>[2]</sup>. Recent researches indicate that defect states existing at the surface and interfaces constitute the primary source of efficiency loss and instability in MHP solar cells (PSCs).

Nickel oxide (NiO<sub>x</sub>) is a well-known inorganic material for use as hole transport layer (HTL) in PSCs, particularly in *p-i-n* configuration. NiO<sub>x</sub> possesses some desirable properties such as a high band gap (>3.6 eV), high optical transmittance, and outstanding stability<sup>[3]</sup>. Despite possessing these desirable properties, NiO<sub>x</sub> suffers from low intrinsic electrical conductivity, a significant amount of surface (and interface) defect states, and non-optimized energy level alignment at the interfaces with MHP. These shortcomings have a significant impact on the electrical properties of corresponding PSCs and needs to be addressed. One potential approach to overcome these issues is to modify the surface of the NiO<sub>x</sub> layer using organic and inorganic molecules.<sup>[4]</sup>

In this study, we employed photoemission spectroscopy i.e. UPS, XPS, and HAXPES to investigate the properties of NiO<sub>x</sub> surfaces and its adjacent interface with an MHP film. To investigate the surface and interface properties, we examined the impact of UV-ozone (UVO) post-treatment process and various NiO<sub>x</sub> surface modifiers. The surface of as-deposited and UVO treated NiO<sub>x</sub> was modified using three functionalized phosphonic acid molecules: MeO-2PACz, 2PACz, and Br-2PACz<sup>[5]</sup>. The MHP layers of MAPbI<sub>3</sub> with thicknesses of 10 nm and 20 nm were deposited on top of these modified NiO<sub>x</sub> substrates by co-evaporation.



Based on our results, we observed the formation of defect states at the interface of MAPbI<sub>3</sub> and bare NiO<sub>x</sub>, resulting from a redox reaction. This effect was mitigated by introducing the interlayers of organic molecules. Additionally, we found that UV-ozone post-treatment of NiO<sub>x</sub> led to increased surface reactivity, which negatively affects device performance. However, by implementing 2PACz-based molecules, the reactivity of UV-ozone treated NiO<sub>x</sub> was reduced, and grafting these molecules resulted in no defects on the NiO<sub>x</sub> surface and improved p-type behavior (Figure 1). Furthermore, we observed that the use of MeO-2PACz interlayer resulted in the highest efficiency and performance in the solar cells compared to the reference devices.

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# Expanding the Compatibility of P3HT Hole Transport Layers for Stable Perovskite Solar Cells

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In order for perovskite solar cells to be commercially competitive, attaining robust environmental stability is of the utmost importance. In a standard device stack the material selection for the surface hole transport layer (HTL) is critical, as it will dictate the degree that air and moisture will penetrate into the sensitive perovskite layer. Present high performing devices rely upon the established small molecule: Spiro-OMeTAD due to its well aligned energy levels, high hole mobility and broad compatibility with differing perovskite chemistries and interfacial passivation layers. However, conductive organic polymers offer several advantages over small molecule materials like Spiro-OMeTAD, such as fast intramolecular transport, greater environmental stability, and reduced cost. Poly(3-hexylthiophene-2,5-diyl) (P3HT) is one such polymer, and has been successfully implemented as an HTL in numerous reported perovskite solar cells, attaining efficiencies up to 24.6% [1]. However, typically these high performances rely upon interfacial perovskite treatments to induce favourable P3HT orientation and packing, and thus introduce restrictions on choice of perovskite chemistry or passivation method, that are not present for Spiro-OMeTAD. While reports that rely on oxidative dopants such as F4TCNQ, to increase the conductivity of P3HT HTL, exhibit lower efficiencies [2]. Therefore, presently P3HT based devices lag behind their Spiro-OMeTAD counterparts, in terms of performance, and versatility. Recently the novel “ion-modulated radical doping strategy” for Spiro-OMeTAD based HTLs has outlined a doping strategy that relies upon a stable radical (Spiro2+TFSI) to increase conductivity, in conjunction with an ionic modulator (TMBP-TFSI) to improve hopping transport between molecules [3]. Drawing inspiration from this report, this work aims to develop an analogous co-doping approach, for P3HT (or other low-cost polymers). By screening oxidising dopants such as charge transfer materials, Lewis acids, photo-initiator salts, and electrophilic salts, in combination with various ionic modulators, to develop a low cost and ubiquitous P3HT based HTL for efficient, stable and inexpensive perovskite solar cells.

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# Reversible Thermochromic Self-trapped Excitonic Emission in One Dimensional Tin-based Halide Perovskite Thin Film

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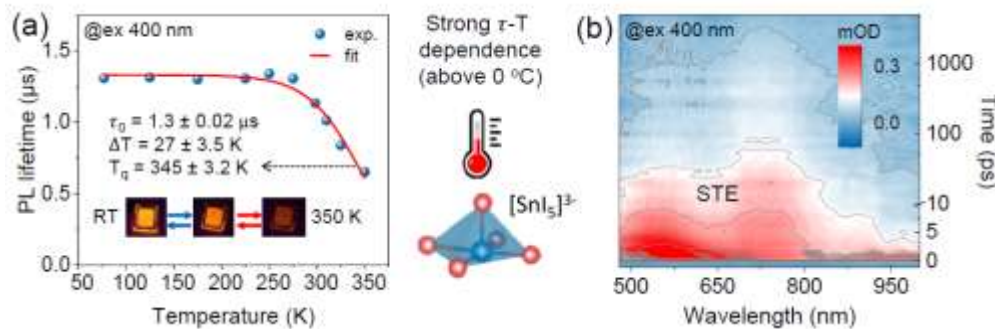
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Lead-free halide perovskites showing self-trapped exciton (STE) emission has aroused great interest in optoelectronics because of the large Stokes shift, broad bandwidth as well as high luminescence efficiency. The STE emission can also exhibit strong temperature-dependence of photoluminescence (PL) lifetime and intensity suggesting a possible application of such material for remote thermography. Recently, thermochromic metal halides based on Sb or Sn has been reported aiming at achieving high-resolution remote thermography, however, the STE-based lead-free halide perovskites showing UV-visible (UV-vis) absorption and high thermal sensitivity of PL lifetimes above 0 °C are still rare. Herein, we designed an efficient and stable one-dimensional tin-based halide perovskite, allowing UV-vis excitation and exhibiting reversible STE thermochromism. The PL lifetime dramatically decreases with higher temperature (above 0 °C) governed by thermally assisted de-trapping process of STE, ensuring its potential for low cost and high-resolution remote thermography. Furthermore, the underlying exciton dynamics are also uncovered by femtosecond transient absorption spectroscopy for comprehensive understanding of STE emission in tin-based perovskite thin film. These findings provide valuable insights and guidance for developing novel lead-free metal halides with STE emissions to realize low cost and high-resolution thermal sensing applications.



**Figure 1. (a) Lifetime-temperature dependence and corresponding Boltzmann-Sigmoid fits with fitting parameters. (Inset: the optical images at different temperatures for one heating-cooling cycle) (b) Pseudocolor representation fs-TA spectra ( $\lambda_{\text{ex}}=400 \text{ nm}$ ) at excitation intensity of  $2.2 \times 10^{15} \text{ photon/cm}^2/\text{pulse}$ .**

# Defect passivation of 2D tin perovskites for lasing applications

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Two-dimensional metal halide tin perovskites are emerging as promising materials for laser gain mediums due to their favorable characteristics, such as significant exciton binding energy, narrow exciton emission, enhanced structural stability, and low defect density. This potential has been demonstrated in laser applications [1]. However, despite these advantages, the absolute photoluminescence quantum yield (PLQY) of 2D perovskites remains relatively low, and the amplified spontaneous emission (ASE) experiences notable quenching with rising temperatures. The exact causes of these limitations are still debated, but it is likely that strong exciton-phonon coupling and the creation of multiple types of defects may play a role by inducing non-radiative losses through trap-mediated processes. Nonetheless, there is a limited understanding of the defect physics in low-dimensional perovskites and a lack of effective strategies for defect their passivation.

To address this, we investigated the impact of the templating organic cation as well as the use of different additives, specifically triphenylphosphine oxide (TPPO) and 1,4,7,10,13,16-hexaoxacyclooctadecane (18-crown-6), in order to passivate the defects, present in the material and to enhance the luminous efficiency. We find that 4-fluorophenethylammonium (F-PEA), characterized by fluorine substitution on the para position of PEA, and the use of the additives for defect passivation yield perovskite films with higher luminescence efficiency, lower ASE threshold, and improved ASE slope efficiency, indicating new synthetic strategies to further improve the material for lasing applications.

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# Unraveling the Defects Passivation During Perovskite Vacuum Co-deposition by In-situ Grazing-Incidence X-ray Scattering and Photoluminescence

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Due to their excellent optoelectronic properties, low cost, and ease of processing, metal halide perovskites (PVSKs) have attracted considerable interest in the past decade. Nevertheless, the performance of PVSK optoelectronic devices is limited by the presence of defects that induce unfavorable charge carrier recombination in the PVSK layers, and various passivation methods have been investigated [1,2]. Consequently, it is imperative to understand the processes of perovskite growth and passivation mechanisms in order to push the limits of their high efficiency.

In this work, we present a detailed study of the evolution of both opto-electronic properties and the structure of PVSK thin films during vacuum co-deposition of methylammonium lead iodide (MAPbI<sub>3</sub>). We introduce potassium chloride (KCl) as a third precursor to passivate defects formed during the deposition. We simultaneously measure *in-situ* grazing incidence wide- and small-angle X-ray scattering (GIWAXS and GISAXS) and photoluminescence (PL). The non-monotonic nature of the PL emission evolution during the growth, with an initial PL emission increase followed by a decay, reflects the formation of defects at the grain boundaries [3]. We observe the direct influence of the introduction of KCl during deposition on the luminescence and, thus, the quality of the material. We believe that such a combined real-time study could be a powerful approach for the optimization of additives and agents for the selective passivation of defects.

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# Where does the current flow? – Spatial inhomogeneity of the reverse bias current and its impact on degradation

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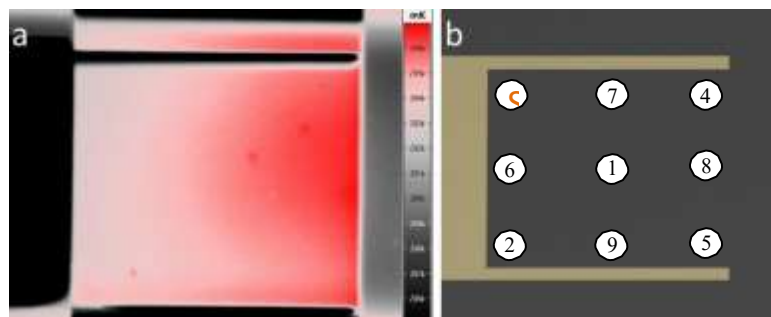
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Before large scale commercialization of perovskite PV is possible, there are still some hurdles to be overcome. The lacking long-term stability is considered as one of the major challenges [1], [2]. Among typical causes of degradation like contact with oxygen or water, the issue of partial shading with the resulting reverse bias stands out since it cannot be solved by better encapsulation [2].

Previous results hint towards the current being the driver behind reverse bias degradation [3]–[6]. It follows that degradation occurs where a reverse bias current flows. In the case of a spatially inhomogeneous current flow, we therefore expect a spatially inhomogeneous impact on the efficiency. Not heeding this can lead to wrong conclusions when reverse bias degradation is investigated.

In order to identify the reverse bias current paths, we use an infrared camera that detects the local heating caused by power dissipation in the cell during the injection of a realistic reverse bias current. An example of thus detected inhomogeneous current flow is displayed in Fig 1a. EQE mapping (procedure schematically depicted in Fig. 1b), EL and PL imaging, and laser-beam induced current (LBIC) mapping are used to visualize local changes in opto-electronic properties. Then, local current flow can be correlated with the local material changes that are accompanying reverse bias degradation.



**Figure 1 (a) Thermographic image of a perovskite solar cell while a reverse bias current is injected, showing spatially inhomogeneous heating. (b) Schematic of a solar cell with gold fingers; the white circles mark the measurement spots for EQE mapping.**

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# Development of Perovskite Absorbers for Application in Perovskite/Perovskite/Silicon Triple-Junction Solar Cells

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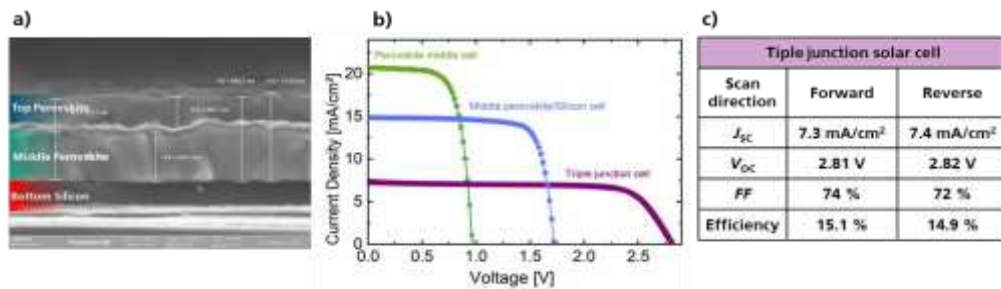
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Within eight years of development, perovskite/silicon dual-junction solar cells have shown remarkable improvement in power conversion efficiency (*PCE*) of up to 33.2% [1]. By addition of a third junction even further enhancement of *PCE* is possible. To achieve the highest *PCE* in a perovskite/perovskite/silicon triple junction solar cell, the right combination of bandgaps should be coupled. In this work, we address some of the main challenges to realize such solar cells. We study the effect of bandgap tuning of the wide-bandgap perovskite top cell on the performance of our triple junction solar cells. In particular, the double-cation perovskite composition  $\text{FA}_{0.75}\text{Cs}_{0.25}\text{Pb}(\text{I}_{0.60}\text{Br}_{0.40})_3$  and triple-cation perovskite composition with general formula of  $\text{Cs}_{0.05}(\text{FA}_{1-x}\text{MA}_x)_{0.95}\text{Pb}(\text{I}_{1-x}\text{Br}_x)_3$  for bandgaps range of 1.78-1.85 eV are investigated. The final device using an optimum composition with 1.83 eV bandgap as top cell shows improved  $V_{oc}$  and  $j_{sc}$ . Furthermore, regarding the perovskite middle solar cell, we report on a high-quality 600-nm-thick 1.55 eV bandgap absorber layer with increased grain size via incorporation of an additive into the perovskite precursor solution. In a next step, thickness and band gap adaption of the perovskite sub-cells is guided by optical simulation. We present our first device with a *FF* of 74%,  $j_{sc}$  of 7.3  $\text{mA}/\text{cm}^2$ , *PCE* of 15.1% and  $V_{oc}$  of 2.8 V which is the highest reported  $V_{oc}$  for this structure so far.



**Figure 1: a) Cross sectional scanning electron microscope image of triple junction solar cell, b) Current density–voltage ( $jV$ ) curves of the middle perovskite single-junction solar cell, middle perovskite/silicon dual-junction solar cell, and perovskite/perovskite/silicon triple-junction solar cell. c)  $jV$  parameters of triple-junction solar cell.**

Acknowledgement: This work was partially supported by the European Union through the Horizon Europe project Triumph under the number 101075725 and the German Federal Ministry for Economic Affairs and Climate Action (BMWK) under contract number 03EE1132A (RIESEN).

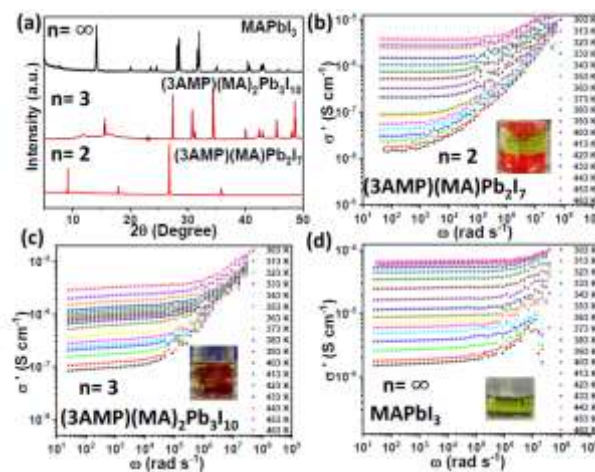
# Spacer Layer Dependent AC conductivity of Two-dimensional Dion-Jacobson Halide Perovskites

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Hybrid organic-inorganic halide perovskites with three-dimensional (3D)  $AMX_3$  structures are impressive semiconducting materials that can be utilized for a wide range of applications such as photovoltaic devices, light emission, detection, and lasing [1]. However, the chemical instability of these perovskites, particularly towards moisture, remains a major impediment to future commercialization. Two-dimensional (2D) Dion- Jacobson (DJ) perovskite structures have emerged as a possible solution to this issue [2].

We have synthesized single crystals corresponding to  $MAPbI_3$  ( $n=\infty$ ),  $3AMP(MA)Pb_2I_7$  ( $n=2$ ), and  $3AMP(MA)_2Pb_3I_{10}$  ( $n=3$ ), where  $n$  is the number of spacer layers. We investigated the structural properties of DJ halide perovskites using XRD. We further analyzed their AC conductivity and dielectric properties, focusing on how it changes with  $n$  increasing 2 to 3 and then to  $\infty$ .



**Figure 1: (a) XRD pattern, and AC conductivity of (b)  $3AMP(MA)Pb_2I_7$  ( $n=2$ ), (c)  $3AMP(MA)_2Pb_3I_{10}$  ( $n=3$ ), and (d)  $MAPbI_3$  ( $n=\infty$ ) DJ perovskites**

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# Exploring the Energetic Landscape of Mixed Iodine-Bromide Perovskites

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Mixed halide perovskites are of great interest for optoelectronic applications due to their high absorption and tuneable bandgap. While their optical properties are well characterised, much remains unknown about the energetic landscape of these materials. By utilizing ultraviolet photoemission spectroscopy (UPS) we explore how compositional engineering of mixed halide perovskites impacts on their electronic structure. We find that varying the Br:I mixing has little impact on the perovskite ionization potential, but has a significant effect of the position of the Fermi level position within the band gap. Specifically, Br-rich perovskites exhibit a p-type character, while I-rich films are n-type. These insights are important for the integration of mixed halide into optoelectronic devices as it would impact the selection of optimal charge extraction/injection layers based on the energetic alignment with the active layer.

# Towards commercialisation with lightweight, flexible perovskite solar cells for residential photovoltaics

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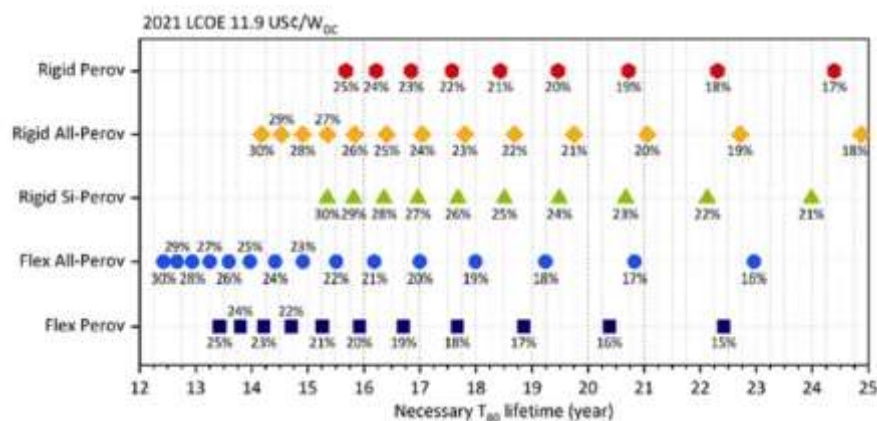
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Here, we assess what lifetimes and efficiencies perovskite solar cells (PSCs) have to reach to lower the price of commercial residential photovoltaic (PV) further. We find that using light and flexible substrates, as opposed to heavy and rigid ones, reduces the total installed system cost of PSCs. The flexibility and lighter weight culminate in a lower balance of systems (BOS) cost, as it is possible to use different mounting methods. This effectively lowers the necessary efficiency or lifetime of PSCs (T80 value) required to achieve the same electricity cost as commercialised silicon. Finally, we extend our analysis toward tandem structures with perovskite-silicon or allperovskite tandem architectures. All results for the 2021 scenario are summarised in Figure 1. For further information please read our publication. [1]



**Figure 4) Comparison of the results for various architectures in the 2021 scenario for residential PV (LCOE of 11.9 US\$/WDC) for a selection of estimated manufacturing costs. The respective indices are the module PCEs.**

[1] M. S. Philippe Holzhey, Michael Prettl, Silvia Collavini, Nathan L. Chang, “Towards commercialisation with lightweight, flexible perovskite solar cells for residential photovoltaics,” Joule, 2023.

# A novel, lead-free halide perovskite derivative for ferro- and piezo- electric applications

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Piezoelectricity is the phenomena of strain-induced electric polarization or vice versa; electric-field induced strain, with applications ranging from actuators, to vibrational energy harvesters. Organic-inorganic hybrid (OIH) ferro- and piezo-electric materials have recently attracted interest over traditional piezo-ceramics due to simpler processing methods, their light-weight nature, mechanical flexibility and lower toxicity compared to traditional ceramics [1,2,3]. Recent reports have shown that by incorporation of a ferroelectric OIH perovskite into a (FA,MA)Pb(I,Br)<sub>3</sub> perovskite solar cell device, and poling it, a higher fill factor and  $V_{OC}$  is achieved via suppression of interfacial recombination due to ferroelectricity-induced modification of the built-in field [4]. Further, molecular ferro- and piezo-electrics often have bandgaps within the optical range, and have thus been studied for their anomalous photovoltaic properties arising from their intrinsic non-centrosymmetry which allows for above-bandgap open-circuit voltage ( $V_{OC}$ ) to be measured [5]. Here, we design a novel, stable lead-free semiconducting hybrid ferroelectric OBI, by inserting a polar, quaternary ammonium organic cation, named 'O' into a face-sharing, BiI<sub>6</sub> anionic framework to form O<sub>3</sub>B<sub>2</sub>I<sub>9</sub> (OBI). OBI crystallizes in a polar space group at room temperature, and exhibits a band gap within the optical range (2.3 eV), in close agreement with that calculated from first-principles methods. Piezoresponse force microscopy (PFM), polarization hysteresis loops and pyroelectric measurements on both single crystals and thin films of OBI reveal its ferroelectric nature, indicating potential applications for flexible self-powered electronics or bio-sensors as well as for ferroelectricity-induced enhancements to the performance of perovskite solar cells.

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- [1] Y.-M. You, W.-Q. Liao, D. Zhao, H.-Y. Ye, Y. Zhang, Q. Zhou, X. Niu, J. Wang, P.-F. Li, D.-W. Fu, Z. Wang, S. Gong, K. Yang, J.-M. Liu, J. Li, Y. Yan, R.-G. Xiong, *Science* (2017), 357, 6348, 306- 309
- [2] S. Wang, A.A. Khan, S. Teale, *Nat Commun* (2023), 14, 1852
- [3] K. Ding, H. Ye, C. Su, *Nat Commun* (2023), 14, 2863
- [4] H. Zhang, Z. Shi, L. Hu, Y.-Y. Tang, Z. Qin, *Adv. Func. Mat.*, (2021), 31, 2100205
- [5] Y. Yuan, T. Li, Q. Wang, J. Xing, A. Gruverman, J. Huang

# Static Moisture induced structural and optical evolution of 2D and 3D perovskites.

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Hybrid perovskites have emerged as one of the most promising materials for optoelectronic applications in the past decade. The photoconversion efficiencies reached around 25.7% for mixed dimensional hybrid perovskites (MDHP). Despite already competing with silicon photovoltaics in efficiency MDHP still lags in long-term stability. Temperature, Moisture, Oxygen, ion migration, and Photoinstabilities leading to Phase segregation are the most known reasons behind the degradation. To tackle the temperature instability larger cation Formamidinium (FA)  $T < 1$  has been introduced with Methylammonium (MA) to improve stability without compromising the PCE. Oxygen instabilities are dealt with by encapsulation and Photoinstabilities have been solved by molecular engineering of Quasi 2D Perovskites. The MDHP has been widely explored for Photovoltaics, LED, and Photodetector applications but recently there have been reports of Hybrid Perovskites (HPV) for Photocatalysis. The Moisture-induced instabilities have been studied widely but not thoroughly which makes the progress in moisture stability slower. In this work, we have studied the hydration of the different Perovskite compositions by in-situ x-ray diffraction and optical measurements to maintain 85% relative humidity (RH). Surprisingly the moisture is seen to degrade the previously reported perovskite composition faster than claimed during the hydration. we also propose the degradation mechanism of 2D/3D perovskites under static moisture condition. This study will help to understand to develop more efficient passivation strategies.

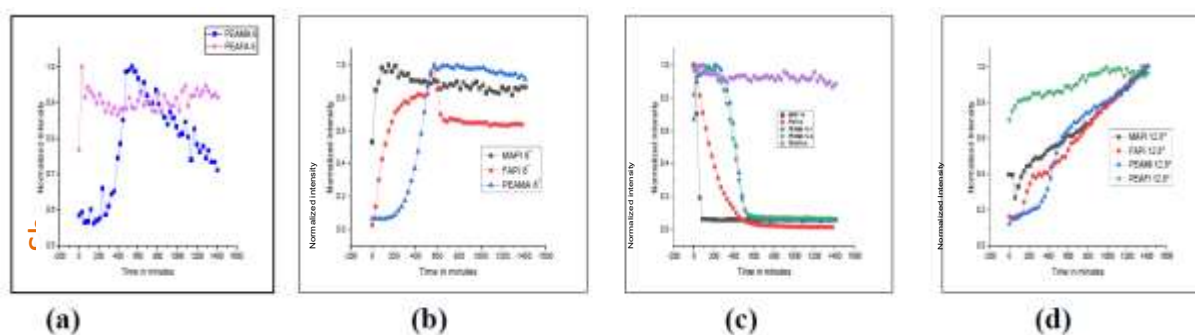


Figure 1 XRD peak evolution of a) PEA b) Hydrated phase of Perovskite c) Perovskite phase d) Degraded phase (PbI<sub>2</sub>) of perovskite phase.

[1] Byranvand, M. M., Otero-Martínez, C., Ye, J., Zuo, W., Manna, L., Saliba, M., Hoye, R. L. Z., & Polavarapu, L. (2022). Recent Progress in Mixed A-Site Cation Halide Perovskite Thin-Films and Nanocrystals for Solar Cells and Light-Emitting Diodes. In *Advanced Optical Materials* (Vol. 10, Issue 14).

# Perovskite-based bifacial and flexible tandem solar cells

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Perovskite (PVSK)-based tandem solar cells including PVSK/Si, perovskite/CIGS, and PVSK/PVSK have recently made great progress, achieving a record power conversion efficiency (PCE) of 33.7% for PVSK/Si tandem. With a high PCE of over 30%, PVSK/Si tandem will account for a significant portion of the solar market with utility- scale use. In particular, bifacial tandem devices based on bifacial Si subcells can further increase power output using additional reflected light. Our group demonstrated a bifacial two-terminal tandem with a high-power output of 29.68 mW cm<sup>-2</sup> under a realistic rear illumination (30 mW cm<sup>-2</sup>) based on bifacial heterojunction Si bottom cells. Meanwhile, PVSK/CIGS thin film tandem devices are more versatile than PVKS/Si tandems, as well as lightweight and flexibility, making them widely applicable to building-integrated PV (BIPV), vehicle-integrated PV (VIPV), and aerospace-PV. Our group developed a facile lift-off process for flexible CIGS solar cells and realized a lightweight and flexible PVSK/CIGS tandem cells, achieving an efficiency of 23.64% (certified: 22.8%), which is one of the highest efficiencies among the flexible PVSK/CIGS tandems.

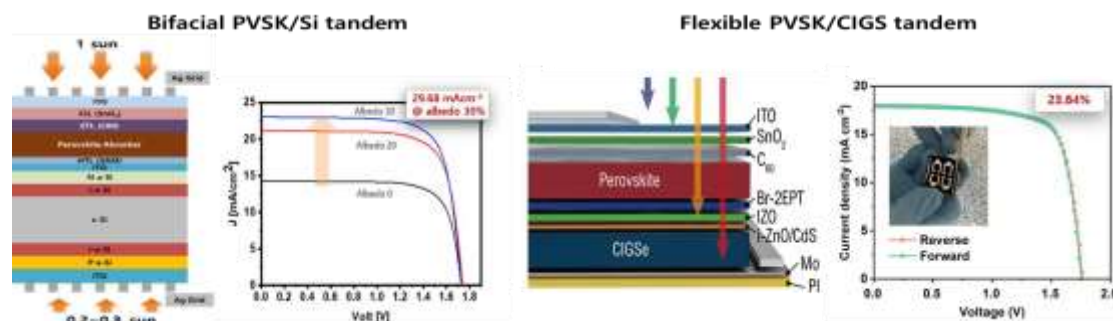


Figure 1 Bifacial PVSK/Si tandem (left) and flexible PVSK/CIGS tandem (right)

[1] S. Mariotti, E. Köhnen, and S. Albrecht, *Science* (2023), 381, 63

[2] M. Jošt, E. Köhnen, A. Al-Ashouri, S. Albrecht, and M. Topič, *ACS Energy Lett.* 2022, 7, 1298

[3] R. Lin, Y. Wang, Q. Lu, and H. Tan, *Nature* 2023, DOI: 10.1038/s41586-023-06278-z

[4] M. A. Green, E. D. Dunlop, M. Yoshita, N. Kopidakis, K. Bothe, G. Siefer, X. Hao, *Prog. Photovoltaics Res. Appl.* 2023, DOI: 10.1002/pip.3726

# FAPbI<sub>3</sub>-based perovskite thin film using Co-evaporation method

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Methylammonium lead iodide(MAPbI<sub>3</sub>) and Formamidinium lead iodide(FAPbI<sub>3</sub>) are well-known perovskite materials with an ABX<sub>3</sub> crystal structure. Research on utilizing FAPbI<sub>3</sub> with a bandgap of 1.47 eV to absorb a wider range of the solar spectrum has been actively conducted. FAPbI<sub>3</sub>-based perovskites have relative advantages in terms of phase stability, thermal resistance, and humidity resistance compared to MAPbI<sub>3</sub>. There are various widely known methods for the fabrication of perovskite films. In most solution-based perovskite film fabrication processes, the use of toxic solvents can be avoided. Additionally, the issue of solvent dewetting, which hinders smooth film formation, is eliminated. This allows for uniform and large-area film formation on rough surfaces or various substrate surfaces, making it suitable for future tandem integration with other solar cell technologies such as silicon or CIGS. We deposited FAPbI<sub>3</sub> films using a co-evaporation method, and optimized the film thickness and heat treatment. UV-vis and PL analysis confirmed the presence of a peak at 803nm wavelength, indicating the absorption and emission properties of the  $\alpha$ -phase FAPbI<sub>3</sub> perovskite film. XRD analysis further confirmed the presence of (001) and (002) crystal planes in the film. The use of vacuum co-deposition for FAPbI<sub>3</sub> deposition allows for excellent uniformity and thickness control, leading to optimized film thickness. In this study, we manufactured a perovskite solar cell by combining the co-deposited FAPbI<sub>3</sub> perovskite with an inorganic charge transport layer using atomic layer deposition. Vacuum co-deposition for FAPbI<sub>3</sub>-based perovskite is expected to have promising effects for the application of tandem perovskite-Si solar cells, making it a potential candidate for next-generation solar cell technologies.

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[1] A. Author, B. Author and C. Author, *Journal* (Year), Volume, pages. M. Liu, M.B. Johnston, H.J. Snaith, Efficient planar heterojunction perovskite solar cells by vapour deposition, *Nature*. 501 (2013) 395–398.



# Alumina nanoparticle interfacial buffer-layer for narrow bandgap perovskite solar cells

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Mixed lead-tin (Pb:Sn) halide perovskites are promising absorbers with narrow bandgaps (1.2-1.3 eV) suitable for high-efficiency all-perovskite tandem solar cells.[1] Currently, the highest efficiency Pb:Sn perovskite solar cells (PSCs) employ methylammonium (MA) as an A-site cation. However, MA is known to be thermally and chemically less stable than formamidinium (FA), therefore it would be favourable to have an MA-free Pb:Sn PSCs that could also deliver high efficiency.[2] Additionally, the solution processing of thick Pb:Sn perovskite films is notoriously difficult in comparison with their neat-Pb counterparts. This is partly due to the rapid crystallization of Sn-based perovskites, resulting in films that have a high degree of roughness. It is more difficult to coat conformal subsequent layers using solution-based techniques on top of rougher films, leading to contact between the absorber and the top metal electrode in completed devices, resulting in a loss of VOC, fill factor, efficiency and stability.[3] Here, we investigate the impact of adding a non-continuous thin layer of alumina nanoparticles inserted in between the thick, rough Pb:Sn perovskite films and the electron transport layers (ETL) in a 'p-i-n' device configuration. This approach leads to enhanced conformality of the subsequent ETL. As a result, devices that employ the thin alumina nanoparticles layer achieved a champion maximum power point tracked efficiency of 15.0% versus 10.3% for the champion control device and the steady-state open-circuit voltage was improved from 0.65 V to 0.75 V. Application of the alumina nanoparticles as an interfacial buffer layer also results in highly reproducible Pb:Sn solar cell devices whilst simultaneously improving device stability at 65 °C under 1 sun illumination at open-circuit condition. Aged devices showed a 6 fold improvement in stability over pristine Pb:Sn devices, increasing their lifetime to 120 hours.

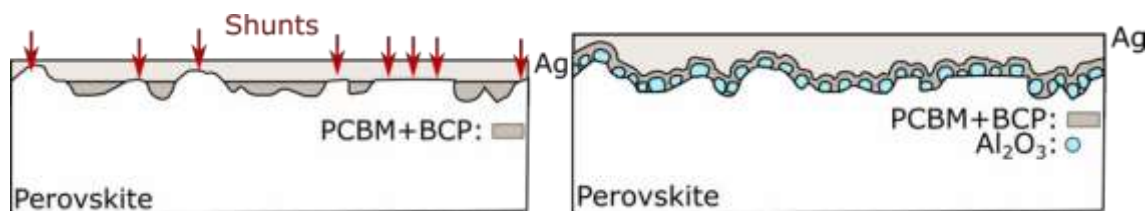


Figure 1 Schematic figures of how a PCBM layer deposits on a rough mixed Pb:Sn perovskite layer without and with Al<sub>2</sub>O<sub>3</sub>.

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# Development of luminescent halide perovskite films through CSS

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Lead halide perovskites have recently emerged as promising low-cost candidates for many optoelectronic applications, including perovskite light-emitting diodes (PLEDs). Among different compositions, 2D or quasi-2D systems exhibit outstanding optical properties, given their inherent quantum-well structure and large exciton binding energy, which results in high photoluminescence quantum yields (PLQYs). Despite the vast majority of PLEDs rely on solution processed thin films, vacuum deposition is a solvent-free and scalable alternative that could have superior control over film thickness and composition.<sup>[1]</sup> Yet, vacuum deposited low dimensional perovskites are still rare given the instability of ammonium salts under heat and high-vacuum conditions.

Here, we report a 2-step solvent-free deposition method using a low-vacuum close-space sublimation (CSS) tool. Given that the distance between the source and the substrate is very small (<5mm), this technique requires very low vacuum conditions, allowing the use of alternative, instable ammonium salts. Starting from a thermally evaporated precursor film, we investigate state-of-the-art 3D compositions and their PL properties after incorporating several surface passivates. Similarly, luminescent 2D and quasi-2D systems based on benzylammonium-FABr lead bromide have been investigated. Interestingly, we observe fast deposition and a high perovskite conversion rates for most of the systems, which are highly dependent on the sample temperature and chamber pressure. In addition, the quasi 2D system does not evolve into different  $n$  dimensionalities with the incorporation of FABr, but it rather segregates into two defined systems with independent PL, providing a stable and defined light emission spectra.

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# Dimethylammonium-incorporated mixed halide perovskite nanocrystals for stabilized red emission

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Ashley Marshall,<sup>2</sup> Bernard Wenger<sup>2</sup> and Henry J. Snaith<sup>1</sup>

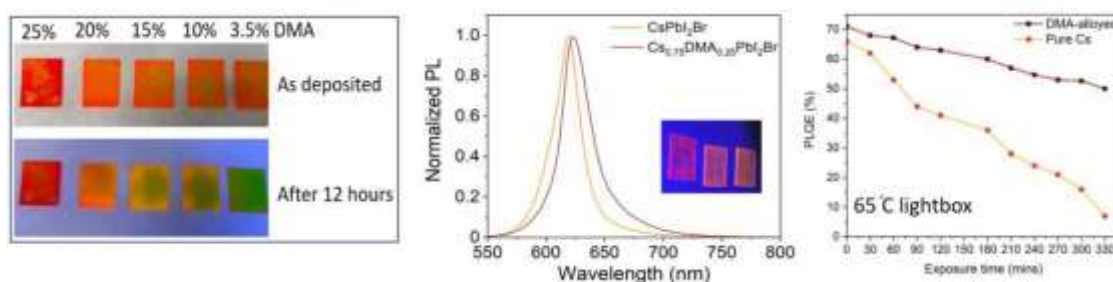
<sup>1</sup> Clarendon Laboratory, University of Oxford, Oxford, OX1 3PU, United Kingdom.

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All-inorganic perovskite nanocrystals are attractive candidates for light emission applications. Of these, cesium lead iodide (CsPbI<sub>3</sub>) nanocrystals have been shown to be promising but their device application is still inhibited by their inherent ambient instability due to rapid conversion of the metastable black perovskite  $\gamma$ -phase into the yellow  $\delta$ -phase at room temperature [1]. With addition of bromine (Br), CsPbI<sub>x</sub>Br<sub>3-x</sub> nanocrystals are formed with ideal bandgaps for emission within the Rec 2020 colour gamut. Furthermore, in contrast to the pure-iodide compositions that require high temperature-based (hot injection) processes to form the perovskite phase, mixed-halide nanocrystals afford facile synthesis through room-temperature ligand assisted reprecipitation (LARP). However, these materials are still plagued by phase separation under optical or electrical excitations of intensities typical in a working device [2].

In this work, we try to alloy the A-site of the pure-red emitting CsPbI<sub>2</sub>Br with dimethylammonium (DMA) to improve its phase stability under excitation while retaining high photoluminescence quantum yields. DMA, among other organic cations, has recently been shown to alloy successfully with Cs in 3D perovskite thin films and lend it stability under operational conditions [3]. To our knowledge, this is the first study of DMA-alloying through facile LARP synthesis techniques. We propose a novel synthetic route at room temperature and then study the crystal structure and morphology as a function of different DMA contents through an interplay of crystallographic and optical data. We report higher ambient stability even under intense optical excitation.



**Figure 1. (Left to right) Stability of films (with varying DMA contents) when left in ambient conditions for 12 hours, photoluminescence (PL) spectra of DMA-containing vs. pure Cs-based nanocrystals and stability tracking through intermittent PL quantum yield measurements on DMA vs. pure-Cs based nanocrystals left at constant 1 sun excitation under white light in a 65°C lightbox.**

[1] G. E. Eperon *et al.*, *J Mater Chem A Mater* (2015), 3, 39.

[2] M. C. Brennan, S. Draguta, P. V. Kamat, and M. Kuno, *ACS Energy Lett* (2018), 3, 1.

[3] A. R. Marshall *et al.*, *Solar RRL* (2021), 5, 1.

# Development of n-type self-assembled monolayers for performance enhancements of perovskite solar cells

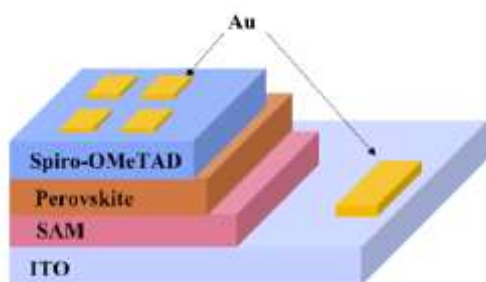
Masahiro Kashiwazaki<sup>1,2</sup>

Takashi Funaki<sup>2</sup>, Kohei Yamamoto<sup>2</sup>, Hiroyuki Yaguchi<sup>1</sup>, Takuro N. Murakami<sup>2</sup>

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We investigated the electron transport layer (ETL) of perovskite solar cells (PSCs) using a self-assembled monolayer (SAM) that can be formed at low temperatures. SAMs ETL does not need to be controlled the film thickness because of adsorption methods and can be applied to the Roll-to-Roll process. n-type organic semiconductor naphthalimide derivatives with anchoring group were used as the basic structure, and the molecules with different substituents on the naphthalimide unit were synthesized. The solar cells performance of PSCs as shown in Figure 1 with different ETLs were compared. ITO glass was used as the transparent conducting film and SAM as the electron transport layer. Triple cation (including methylammonium, formamidinium, and cesium) mixed halide perovskite crystals were used as the light absorption layer. Spiro-OMeTAD was used as the hole transport layer. Au was used for the electrode. Figure 2 shows the  $J-V$  characteristics of the PSCs with SAM that obtained as the highest efficiency. It is expected that changing the different orientation to the substrate and affinity to perovskite will affect on the performance enhancements of the solar cells. The relationship between molecular structure of the SAMs and the performance of the solar cells are discussed in this presentation.



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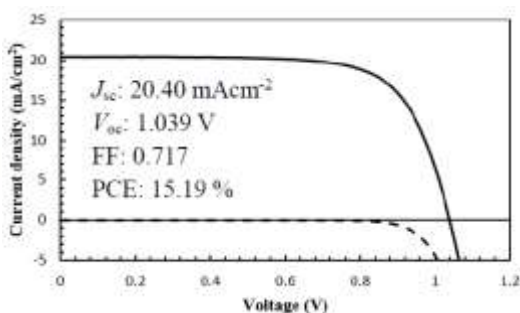


Fig 2. J-V characteristics of PSC

# Light Makes Right: Laser Polishing for Surface Modification of Perovskite Solar Cells

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Interface engineering is a common strategy for passivating surface defects to attain open circuit voltages (Voc) in perovskite solar cells (PSCs). In this work, we introduce the concept of polishing a perovskite thin-film surface using a nanosecond (ns) pulsed ultraviolet laser to reduce surface defects, such as dangling bonds, undesirable phases, and suboptimal stoichiometry. A careful control of laser energy and scanning speed improves the photophysical properties of the surface without compromising the thickness. Using laser polishing, a Voc of 1.21 V is achieved for planar PSCs with a triple cation composition, showing an improved perovskite/hole transport interface by mitigating surface recombination losses. We measure an efficiency boost from 18.0% to 19.3% with improved stability of up to 1000 h. The results open the door to a new class of surface modification using lasers for interface passivation in well-controllable, automated, scalable, and solvent-free surface treatments.



**Figure 1: A selective area ablation of perovskite thin film to obtain semi-transparency in the visible using a pulsed laser.**

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[1] "Light Makes Right: Using Laser Polishing for Surface Modification of Perovskite Solar Cells" Kedia, Mayank; Rai, Monika; Phirke, Himanshu; Aranda, Clara ; Das, Chittaranjan; Chirvony, Vladimir; Boehringer, Stephan; Kot, Malgorzata; Malekshahi Byranvand, Mahdi; Flege, Jan Ingo; Redinger, Alex; Saliba, Michael (<https://pubs.acs.org/doi/10.1021/acseenergylett.3c00469>)

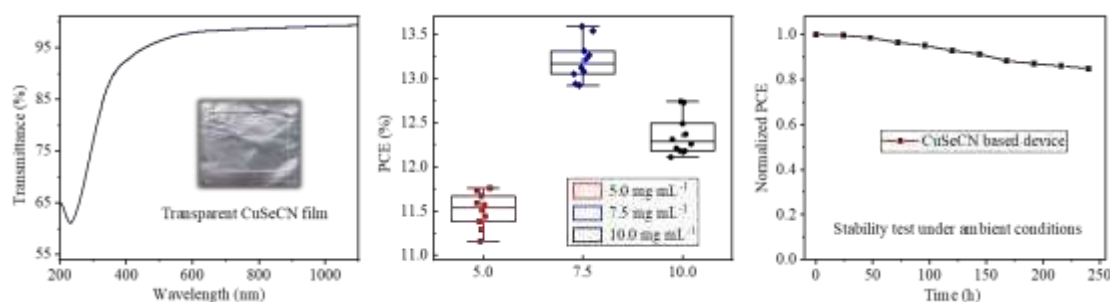
# Copper(I) selenocyanate: A Solution-processed Hole Transport Layer for Organic and Perovskite Solar Cells

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Asit Patra

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Inorganic hole transport layers (HTLs) have emerged at the forefront for solution-processable excitonic devices due to high chemical stability, hole mobility and low fabrication cost. Herein, we have successfully fabricated CuSeCN as an efficient hole transporting layer which possesses high optical transparency (>94%), high work function (~5.1 eV), solution processability, low processing temperature, making it an ideal candidate as an HTL. We proposed a new HTL modification by utilizing CuSeCN processed from eco-friendly and inexpensive solvents as a novel alternative to conventional n-alkyl sulfide solvents. Recently, we have reported DMSO and DMF solvents for solution-processable deposition of CuSeCN films for the fabrication of organic bulk heterojunction solar cells, with a simple device architecture ITO/CuSeCN/PCDTBT:PC<sub>71</sub>BM/Al. An average power conversion efficiency (PCE) was achieved up to 4.03% using DMF as deposition solvent.[1] To further elucidate its potential as an efficient hole extracting layer, inverted planar perovskite solar cells has been fabricated with device architecture ITO/CuSeCN/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>/PC<sub>61</sub>BM/BCP/Ag and obtained the maximum PCE of 13.59% ( $V_{oc} = 0.99$  V,  $J_{sc} = 18.8$  mA/cm<sup>2</sup> and FF = 0.73).[2] In this, a transparent CuSeCN layer is processed from low-temperature aqueous ammonia processed CuSeCN via spin-coating in ambient air. To the best of our knowledge, this is the first demonstration of high-performance solution-processed excitonic devices where CuSeCN is deposited from a solvent that is compatible with flexible and large area applications. Thus, the successful incorporation of CuSeCN as an efficient HTL pave the way for the development of high-performance HTLs for excitonic solar cells as well as for other optoelectronic devices.



**Figure 1 a) Transmission spectrum of CuSeCN film. b) Perovskite solar cells performance is strongly affected by the concentration of CuSeCN solution. c) The long-term stability of the optimized CuSeCN-based perovskite device without encapsulation in the ambient environment.**

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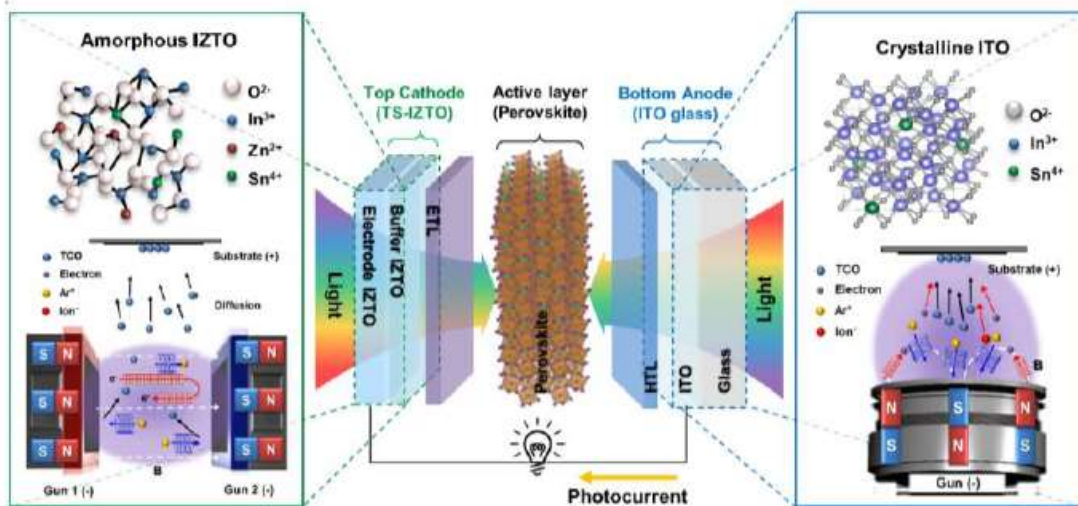
# Plasma damage-free deposition of transparent top cathode using linear facing target sputtering for semi-transparent perovskite solar cells

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In this study, we present our findings on high-performance semi-transparent perovskite solar cells (PSCs) designed for use in building-integrated photovoltaics (BIPV). We used bidirectional transparent electrodes composed of a typical magnetron sputtered InSnO (ITO) anode and a low energy sputtered InZnSnO (IZTO) cathode to fabricate the PSCs [1]. By employing a two-step sputtering process, consisting of the sequential sputtering of a thin buffer layer and then a thick, dense IZTO layer, we were able to produce a transparent IZTO cathode for a p-i-n planar type PSC without any plasma damage. Compared to PSCs with an ITO cathode prepared by typical DC magnetron sputtering, the PSC with the two-step sputtered IZTO cathode demonstrated significantly higher power conversion efficiency (PCE) of 15.52%, as opposed to 3.43%. This improvement was due to the absence of plasma damage. The PCE of the semi-transparent PSC with IZTO cathode was comparable to the PCE (17.04 %) of an opaque PSC with an opaque Ag cathode, demonstrating that the two-step linear facing target sputtering (FTS) process is a feasible approach to producing high-quality transparent top cathodes for semi-transparent PSCs. For mass-production of semi-transparent PSCs for BIPV, FTS-based two-step sputtering has great potential to become a key technique for producing smart windows, which can replace typical solution coating or other complicated transfer processes. This study shows that bidirectional transparent electrodes, coupled with the two-step sputtering process, can significantly enhance the performance of semi-transparent PSCs, making them a promising technology for BIPV applications.



**Figure 1** Schematic structure of semi-transparent PSC with crystalline ITO anode grown by DC magnetron sputtering and amorphous IZTO cathode grown by co-sputtering of ITO and IZO targets using linear FTS.

[1] S.-H. Lim et al., *Nano Energy* (2021), 82, 105703.

# Study on Charge Carrier Transport in HTL via Optoelectronic Analysis

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Perovskite solar cells (PSCs) have emerged as a potential candidate to produce state-of-the-art highly efficient (over 26% power conversion efficiency)[1], and low-cost device manufacturing. However, the efficiency of these PSCs is still limited owing to their undesirable non-radiative recombination that is mainly caused by the various trap-states and energy losses because of poor charge-carrier characteristics. Mainly, the state-of-the-art PSCs suffer from either lower mobilities or higher trap-densities. Hole transporting layers(HTLs) can modify by side chain substitution and by changing the length of main chain.[2] So plenty of research is being done on HTL. Therefore, our work presents a comprehensive evaluation of the impact of the mobility, thickness, and doping density of the hole transporting layers(HTLs) for PSCs.[3] Herein, we specifically investigated the impact of the HTLs thickness on the photovoltaic characteristics and charge-carrier dynamics of PSCs through optoelectronic analysis.[4] These analyses are based on the combination of compositional and structural engineering analysis to prepare efficient HTLs of perovskite film.[5] From these analyses, we tried to introduce the basic guidelines for the optimization of HTLs to prepare highly efficient and stable PSCs.

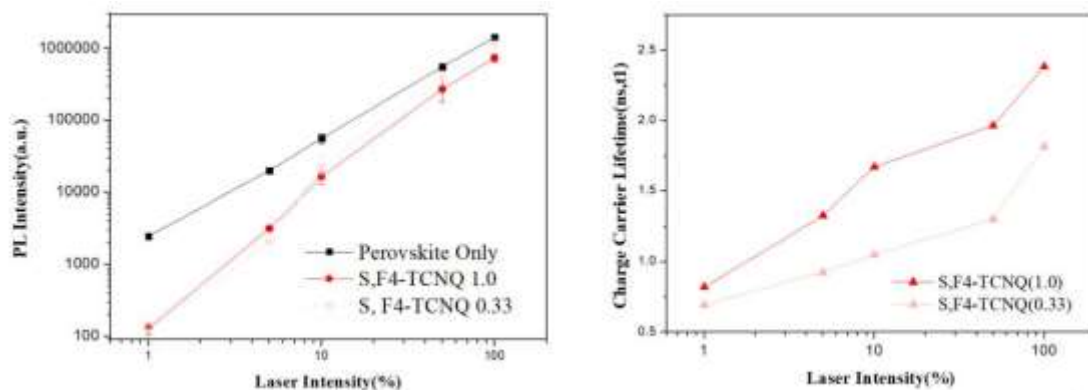


Figure 1. Optoelectronic analysis method by changing light intensity

[1]Park, J., Kim, J., Yun, H., Paik, M. J., Noh, E., Mun, H. J., Kim, M. G., Shin, T. J., & Seok, S. I. *Science*(2023), 616 (7958), 724-730

[2]Moon, S., Khadtare, S., Wong, M., Han, S. H., Bazan, G. C., Choi, H., *Journal of Colloid and Interface Science* (2018), 518, 21–26.

[3]Lee, I., Rolston, N., Brunner, P. L., & Dauskardt, R. H. *ACS Applied Materials and Interfaces* (2019), 11(26), 23757–23764.

[4]Kang, G., Yoon, J. S., Kim, G. W., Choi, K., Park, T., Baek, R. H., Lim, J. *Journal of Materials Chemistry A* (2019), 7(45), 25838–25844.

[5]Chen, X., Guo, B., Zhang, Z., Zhang, B., Zu, X., Ouedraogo, N. A. N., Oh, J., Cho, Y., Odunmbaku, G. O., Chen, K., Zhou, Y., Chen, S., Yang, C., Du, J., & Sun, K. *DeCarbon* (2023), 1, 100004.



# **Modulating Electrical Conductivity of Metal Halide Perovskite Thin Films through Surface Metal Halide Deposition**

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Metal halide perovskites have received a lot of attention in the field of solar cells and light emitting diodes due to their excellent optoelectronic properties. However, despite such interests, electrical doping, which is an intentional tuning of charge carrier density, still remains challenging in metal halide perovskites. Here, we show that the electrical conductivity of methylammonium lead triiodide (MAPbI<sub>3</sub>), a representative 3D perovskite, can be effectively increased by thermally depositing metal halides on the film surface and that the conductivity level can be tunable by varying the amount of the metal halide deposited. This work would be relevant for enabling effective control of electronic structure and energy band alignments within perovskite-based devices.

# Mode locking of hole spin coherences in CsPb(Cl,Br)<sub>3</sub> perovskite nanocrystals generated via positively charged excitons

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The spin physics of perovskite nanocrystals is attracting increasing attention both for fundamental studies and spintronic applications. Here, stable CsPb(Cl<sub>0.56</sub>Br<sub>0.44</sub>)<sub>3</sub> lead halide perovskite nanocrystals embedded in a fluorophosphate glass matrix are studied by time-resolved optical spectroscopy excited via the positively charged exciton transition to unravel the coherent spin dynamics of holes and their interaction with nuclear spins of the <sup>207</sup>Pb isotope [1]. We demonstrate the spin mode locking effect and nuclear induced frequency focusing leading to the synchronization of the hole spin Larmor precession frequencies of the nanocrystal ensemble. Within the spin mode locking effect the spin precession frequencies of a nanocrystal ensemble become locked to harmonics of the driving laser pulse repetition frequency. The spin mode locking was first observed on self-assembled (In,Ga)As/GaAs quantum dots and led to the discovery of various physical phenomena [2]. As one of the main features, analogously to the Hahn echo technique, this effect leads to a recovery of the dephased ensemble spins. Hence, the technique allows to access the homogenous decoherence time T<sub>2</sub>. Further, in the experiments the nuclear induced frequency focusing was observed, whereas due to the hyperfine interaction the nuclear spins get polarized in such a way that they enhance the spin mode locking effect by providing a tiny Overhauser field which tunes the precession frequency of the nanocrystal spins in such a way that they fit the spin mode locking harmonics.

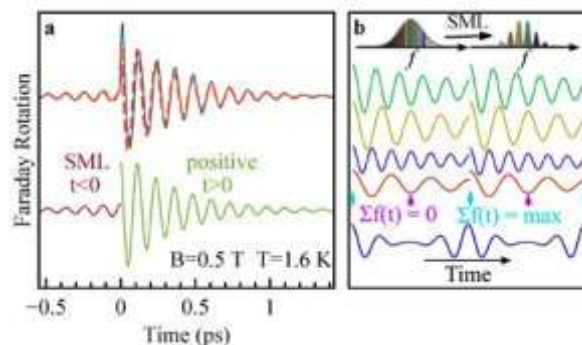


Figure 1: a Spin Mode locking signal in NC, b Spin Mode-locking scheme

[1] Kirstein, E., Kopteva, N. E., Yakovlev, D. R., Zhukov, E. A., Kolobkova, E. V., Kuznetsova, M. S., Belykh, V. V., Yugova, I. A., Glazov, M. M., Bayer, M., Greilich, A. Mode locking of hole spin coherences in CsPb(Cl,Br)<sub>3</sub> perovskite nanocrystals. *Nat. Commun.* 14, 699 (2023).

[2] Greilich, A., Yakovlev, D. R., Shabaev, A., Efros, A. L., Yugova, I. A., Oulton, R., Stavarache, V., Reuter, D., Wieck, A., Bayer, M. Mode Locking of Electron Spin Coherences in Singly Charged Quantum Dots. *Science* 313, 341–345 (2006).

# Using Bayes' Theorem to Evaluate Time-Resolved Photoluminescence Data

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Time-resolved photoluminescence (TRPL) is a powerful technique to probe transient behaviour of charge carriers in semiconductors after photoexcitation. In most reports however, a mono- or biexponential models are used to evaluate the data obtained from TRPL. This is of course a crude model, as it will only allow the extraction of a single lifetime (or two lifetimes) from the data, which doesn't necessarily have a physical meaning. Following a recent report, we attempted using Bayes' theorem to evaluate the TRPL data instead. In this approach all possible parameter combinations are used to simulate TRPL traces and each is assigned a likelihood, which depends on their overlap with the TRPL data. However, this process becomes very time consuming with a larger parameter space. Here, we show an updated method, in which we include a Markov-Chain Monte-Carlo (MCMC) algorithm to explore the n-dimensional parameter space. The computational time is reduced, as not all combinations of parameters need to be simulated, but only the ones with a higher probability of overlapping with the data. This allows us to run this evaluation of the TRPL data on a normal laptop within a few hours. The power of the technique becomes apparent, after we evaluate a set of fluence-dependent TRPL data with up to 11 parameters. For each parameter we obtain a probability distribution as well as a correlation plot with all other parameters. This will be helpful for the investigation of novel and existing materials, as it allows a deeper insight into underlying physics that may have been undiscovered before. We then move on to compare the extracted parameter values with other methods, such as photoluminescence quantum yield (PLQY) or transient photoconductivity (TPC). Overall, we show that this method of evaluating data can be extremely powerful, as it won't be limited by 'overfitting' and in the case of TRPL allows the extraction of a variety of fundamental parameters from just a simple optical measurement.

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[1] C. Fai, et.al; Joule, 2022, 6, 11, 2585.

# Atmospheric neutron resilience of flexible perovskite solar cells with thoughtfully designed organic hole transport material

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Flexible perovskite solar cells (f-PSC) are excellent candidates for space applications, thanks to record efficiencies of 23.4% [1], close to the 26% record reached by rigid devices [2], and excellent power densities as high as 29 W/g [3].

Our previous work in Hole Transport Material (HTM) optimization revealed the positive impact of the insertion of benzothiadiazole (BTD) unit on a P3HT scaffold upon neutron irradiation [4]. Here we synthesized two different HTMs in which PTAA is copolymerized with (i) a phenothiazine or (ii) both a phenothiazine and a BTD. As an added value, the new HTMs could be processed in more sustainable solvents than toluene, *i.e.* THF.

Neutrons have shown to induce degradation in the performance of traditional solar cells used in space, however the literature on the matter for PSC is still not as extensive. Studying potential damage sources selectively will help us estimate more accurately the ageing of our devices in space. Therefore here we studied degradation damages induced by atmospheric-like neutrons (fluence of  $5 \cdot 10^9$  n/cm<sup>2</sup>), provided by the Chip-IR beamline in the Rutherford Appleton laboratory, which well represent the environment in Low Earth Orbit [5]. PV characterization of the devices showed that the new HTMs (and especially the BTD-modified one) are a viable alternative to the commercially available PTAA, with improved resilience to atmospheric neutrons. Furthermore, photoluminescence imaging revealed negligible damage in the active perovskite itself, suggesting that the loss in electrical performance is attributable to charge extraction processes and interface degradation.

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[1] Wu et al., *Joule* (2022), 7, 1-18

[2] <https://www.nrel.gov/pv/cell-efficiency.html> (2023).

[3] Saewon Kang, et al., *J. Mater. Chem. A* (2019), 7, 1107

[4] De Rossi et al., *Nanoenergy* 93 (2022) 106879

[5] C. Frost, et al. *Reliability Physics Symposium*, (2009), 952-955

# Developments for the industrialization of graphite-based, in-situ crystallized perovskite solar cells

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The concept of printed mesoporous, monolithic cells with graphite and carbon-based porous electrode layers (c-PSC) has been intensively investigated by various groups on cell and small to medium-sized module scale. Graphite based electrodes offer potential advantages over frequently applied organic hole conductors and metallized electrodes due to their high chemical and electrochemical stability. After having reported a certified, stabilized solar efficiency of 15.4% for c-PSC on cell level [1], we recently reached an efficiency of 18.5% by improving the electron blocking characteristic at the interface between the perovskite and the graphite electrode using an 3D-2D approach [2]. Another challenge consists in the long-term stable sealing of c-PSC. For this purpose, we developed a method, in which a gas assisted liquified perovskite precursor [3] is crystallized “in-situ” as the final step of the module manufacturing. This allows the use of printable glass solder sealing material and fusing two glass substrates together at a temperature above 600 °C, resulting in a high-quality sealed prefab-module with a homogenous plate distance of 10 µm. Such a module fabrication concept, which benefits from the cost-effective technologies of the glass industry, has been successfully demonstrated by us for large sized dye solar cell modules in the past [4], and since several years is now transferred to the perovskite technology [5]. In this presentation, we give an overview over the processing steps implemented at Fraunhofer ISE with a focus on industrial scalability and report about the inverse temperature crystallization step as monitored by time dependent and potentiostatic photoluminescence imaging [6]. Several methods are currently studied to control the perovskite seeding process in the m-TiO<sub>2</sub> layer. We also report on a novel design of microfluidic channels which are generated via laser assisted glass etching.

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[1] S. Zouhair, B. Luo, D. Bogachuk, D. Martineau, L. Wagner *et al.*, *Solar RRL* (2021), 6, 2100745.

[2] S. Zouhair, S.M. Yoo, D. Bogachuk, J.P. Herterich, J. Lim *et al.*, *Advanced Energy Materials* (2022), 12, 2200837.

[3] D. Bogachuk, L. Wagner, S. Mastroianni, M. Daub, H. Hillebrecht and A. Hinsch, *Journal of Materials Chemistry A* (2020), 8, 9788-9796.

[4] A. Hinsch, W. Veurman, H. Brandt, K. Jensen and S. Mastroianni, *ChemPhysChem* (2014), 15, 1076-1087.

[5] L. Wagner, S. Mastroianni and A. Hinsch, *Joule* (2020), 3, 2463–2471.

[6] L. Wagner, P. Schygulla, J.P. Herterich, M. Elshamy, D. Bogachuk *et al.*, *Matter* (2022), 7, 2352-2364.

# Encompassing Tetrafluoroborate Anion into FAPbI<sub>3</sub> Photoabsorber Layer for Efficient and Stable Perovskite Solar Cells

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FAPbI<sub>3</sub> is a promising photoabsorbing material in perovskite solar cells (PSCs) because of its narrow band gap, which is relatively close to the optimal value for single cells (ca. 1.4 eV). The introduction of different ions into the perovskite material can improve its properties. However, the introduction of monoatomic ions such as Br<sup>-</sup> and Cs<sup>+</sup> broadens the bandgap of FAPbI<sub>3</sub> and reduces its advantage. Meanwhile, molecular ions have the potential to achieve functions that are not attainable by such monoatomic ions. Tetrafluoroborate molecular anion (BF<sub>4</sub><sup>-</sup>) possesses an effective ionic radius of 2.18 Å and it is similar to iodine anion (2.20 Å) so it can be encompassed into perovskite crystal. In particular, it has been reported that incorporation of BF<sub>4</sub><sup>-</sup> can decrease bandgap of perovskite materials and additionally render perovskite hydrophobic [1]. Thus, BF<sub>4</sub><sup>-</sup> is prominent candidate to be introduced into FAPbI<sub>3</sub> crystal. However, the effects of encompassing BF<sub>4</sub><sup>-</sup> are still unclear, such as the narrowed bandgap whether it is derived from the crystal structure change [1,2] and the origin of the resulting hydrophobicity [3]. In the present study, we investigate effects of encompassing BF<sub>4</sub><sup>-</sup> into FAPbI<sub>3</sub>. As the result, using MABF<sub>4</sub> as an additive to FAPbI<sub>3</sub>, the optical bandgap was decreased without crystal structure change. In addition, MABF<sub>4</sub> additive resulted in an enhancement of the photoconversion efficiency (PCE) up to 22.5%. Furthermore, the long-term stability at 303 K with 50% relative humidity was also improved by the BF<sub>4</sub><sup>-</sup> addition likely because the introduced BF<sub>4</sub> moiety endowed perovskite with hydrophobicity. Further details of the effects on these improvements will be discussed to the presentation.

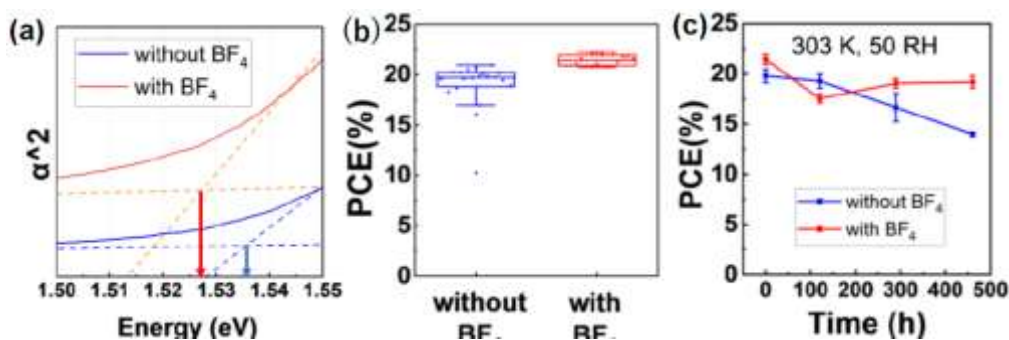


Figure 1 (a) Estimated optical bandgaps, (b) initial PCEs, (c) long-term stability of PCEs

[1]Su et al., *J. Mater. Chem. A* (2023), 11, 6565–6573.

[2]A. Yang et al., *J. Phys. Chem.* (2021), 125, 21223-21233.

[3]N. Nishimura et al., *New J. Chem.* (2023), 47, 4197-4201.

# “Horse measurement” for accurate quantification of information on the charge dynamics in halide perovskites

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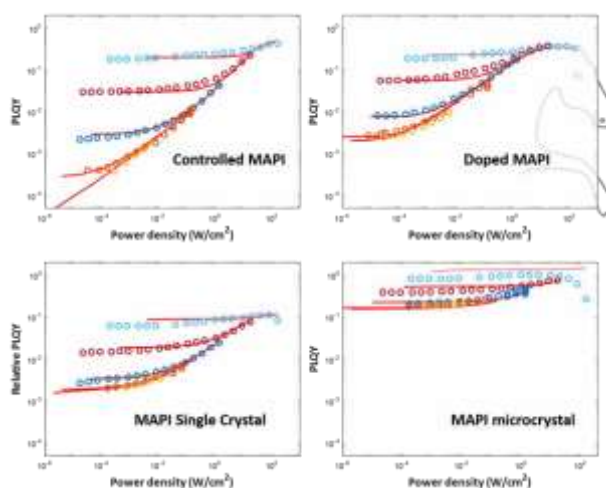
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<sup>2</sup> Indian Institute of Technology Roorkee, Roorkee, 247667, India.

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Owing to their low exciton binding energy, halide perovskites (HPs) have free charge carriers as the majority carriers. The presence of free charge carriers along with charge traps make the photoluminescence quantum yield (PLQY) excitation power dependent. This excitation power dependence of PLQY can be probed with either a continuous wave (CW) LASER or a pulsed laser. We used a pulsed excitation source to study the average excitation power dependence of PLQY, in this case PLQY can be represented as a 2- dimensional function of pulse fluence (P) and pulse repetition rate (f).[1] Alternatively, by calculating the average excitation power density as a function of pulse ‘P’, and pulse ‘f’, PLQY can be plotted similar to a one-dimensional multivalued function. Plotting the data with later scheme lets us identify a recognizable shape, which looks like the mane of a running horse and therefore this way of measurement of PLQY is termed as the “Horse measurement” and the plot of PLQY vs average excitation power density is called “Horse plot”. “Horse measurement” is best suitable for doing deeper shape analysis of PLQY (f, p), as well as fitting the data to a model with a better accuracy. We have measured several different samples of halide perovskite (MaPbI<sub>3</sub>) and just by doing shape analysis we can qualitatively predict about the relative change in charge trapping, defect density, radiative and non- radiative rate constants. We also verified these predictions by fitting the “Horse plot” in the framework of Shockley-Read-Hall+(SRH+).



**Figure 1** Horse plot for different types of MaPbI<sub>3</sub> perovskite samples a) Controlled MaPbI<sub>3</sub>, b) Doped MaPbI<sub>3</sub>(doped with benzylamine), c) MaPbI<sub>3</sub> single crystal, d) MaPbI<sub>3</sub> microcrystal.

[1] A Kiligaridis, et al. Nature Communications 12.1 (2021): 3329.

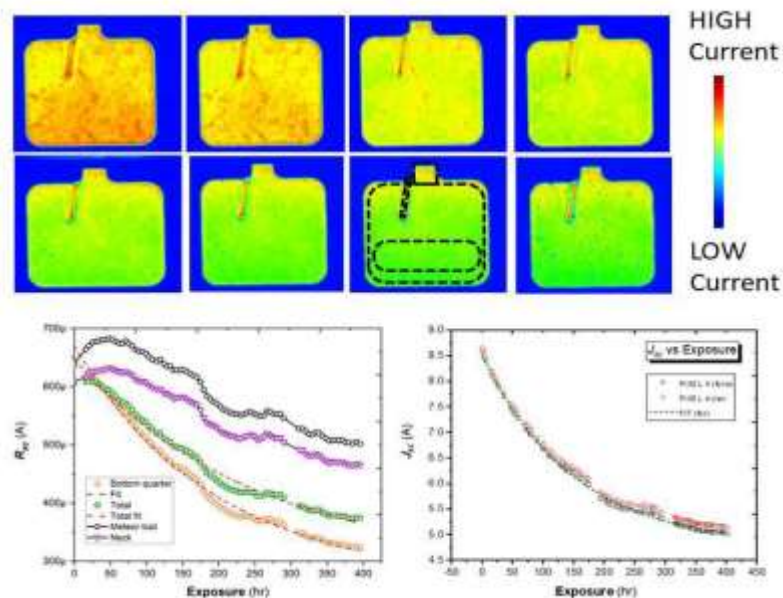
# Coordinated Image and Bulk Electrical Characterisation for Better Elucidating the Role Heterogeneity Plays in Perovskite Solar Cell Degradation

Jamie S Laird<sup>1</sup>

Philippe Holzhey<sup>2</sup>, Pria Ramkissoon<sup>1</sup>, Xinyi Shen<sup>2</sup>, Karl-Augustin Zaininger<sup>2</sup>, David McMeeking<sup>2</sup>, Udo Bach<sup>3</sup>, Henry Snaith<sup>2</sup> and Trevor A Smith<sup>1</sup>

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Challenges facing the commercialization of perovskite solar cells require the development of new testing suites elucidating device degradation and failure. We developed a system that combines a Laser Beam Induced Current microscopy (LBIC) sub-method called Intensity Modulated Photocurrent Spectroscopy (IMPS) Imaging [1] with electrical characterization. Here we describe the method and apply it to follow the heterogeneous degradation of a FA<sub>0.83</sub>CS<sub>0.17</sub>Pb(I<sub>0.6</sub>Br<sub>0.4</sub>) perovskite solar cell (Figure 1), together with  $J_{sc}$  recorded over the same 400 hours exposure to  $\sim 0.8$ SUN. Different areas are seen to degrade or even improve over part of the exposure as opposed to the bulk  $J_{sc}$  measurements highlighting the need for imaging. These heterogeneities can come for example from the charge transport layer [2]. Our results indicate that for stable perovskite solar cells homogenous charge transport layers are required. The system developed and results collected will be discussed in detail.



**Figure 1: (Top) LBIC/IMPS images of the cell from 0 to 400 hrs. (Bottom) (Left) Extracted short-circuit PC from different areas and (right) the degradation in the bulk  $J_{sc}$  over the same period.**

[1] J.S. Laird, S. Ravishankar, et al., *Small Methods* (2022), Volume 6, Issue 8 2200493

[2] A. Dasgupta *et al.*, *ACS Energy Lett.*, vol. 7, no. 7, pp. 2311–2322, Jul. 2022, doi: 10.1021/acsenerylett.2c01094.



# Sustainable and Circular Management of Perovskite Solar Cells via Green Recycling

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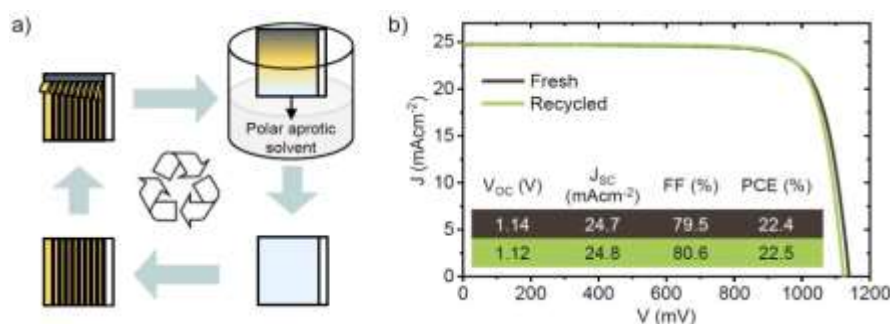
<sup>1</sup> VL, FF, GP, LP, SC, MM, GB, MD, RP, MDB, GG University of Pavia, Via T. Taramelli 14, 27100 Pavia, Italy.

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Material management is responsible for two-thirds of the global greenhouse gas emissions, which renders smart designing of new technologies a crucial strategy to achieve climate neutrality.[1] In the emerging photovoltaic field, perovskite solar cells (PSCs) are gaining attention because of their remarkable efficiencies and reduced levelized cost of electricity.[2] However, in order to introduce them into a circular economy perspective, it is pivotal to conceive a strategy for their end-of-life management.

I will present the recycling of the most environmentally impacting and most expensive component of PSCs, i.e. the transparent conductive oxide (TCO) glass substrate.[3] Through the use of the green solvent dimethyl sulfoxide (DMSO), the upper layers of the device are dissolved up to the metal oxide electron transport layer (ETL), which remains firmly attached to the TCO (Figure 1a).[4] The recovered substrates are employed to fabricate second-generation PSCs, showing the same power conversion efficiency (PCE) as fresh samples (Figure 1b) and proving that the recycling process is with zero losses.



**Figure 1 a) Recycling scheme of perovskite solar cells (PSCs) transparent conductive oxide (TCO) glass substrates. b) Current density – voltage (J-V) characteristics of PSCs fabricated with fresh and recycled TCO glass substrates.**

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# Surface or Bulk Defects - Halide Perovskites Probed by Photothermal Deflection Spectroscopy

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Organic-inorganic halide perovskites (OHPs) thin films and single crystals are highly defect tolerant. These low-temperature solution-processed materials are far from being perfect monocrystals. Moreover, halide elements are able to move in the crystalline lattice, the OHPs surface is highly defective, etc. Despite this, the overall photovoltaic and light emitting properties of OHPs are at a very high level.

The most important factor limiting nowadays OHPs applications is non-radiative recombination. Passivation of a wide variety of defects is one of the main topics in the OHP community. From our recent experiments <sup>[1]</sup> we see the defect evolution during the OHPs film growth. In the beginning, low defects density crystalline grains are growing. Once these grains start to connect, defective grain boundaries are formed. At this stage, the radiative recombination probability decreases, which leads to a reduction of open circuit voltage ( $V_{OC}$ ). We need to find the right passivation strategy to preserve the original properties of the deposited film. For that, we have to understand where these defects are located.

With the help of Photothermal Deflection Spectroscopy (PDS), we will probe the absorption spectra of MAPbBr<sub>3</sub> single crystals. Bismuth doping is used to introduce additional bulk defects in the MAPbBr<sub>3</sub> single crystals. The surface defects will be introduced by the illumination of the crystal by visible light. Both, the absorption spectra and photoluminescence quantum yield (PLQY), are significantly affected by the defects concentration. The main attention will be given to the phase of the measured PDS signal. The significant shape of the phase shift gives us information about the penetration depth of the PDS measurement. The phase shift is increasing when the penetration depth decreases – the thermal signal is taken from the volume nearer to the surface. Based on a measurement under different conditions and computer simulations, we are able to distinguish between defects situated at the surface and homogeneously distributed in the bulk of the probed OHP single crystal.

In this way we are able to localise deep defects in the space. This basic understanding of defects' properties will help us to find the optimal passivation strategy to optimise the perovskite optoelectronic quality.

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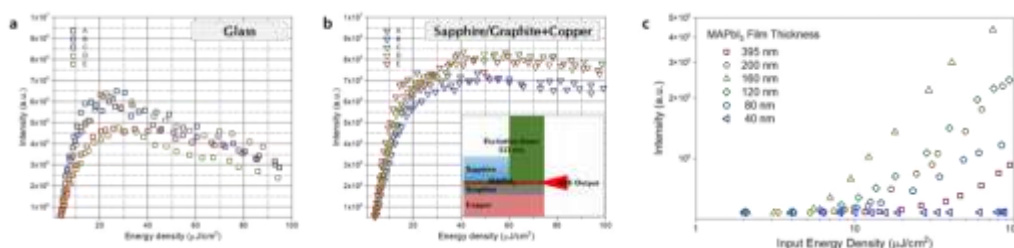
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# Strategies for low threshold and photo-stable amplified spontaneous emission from halide perovskite thin films

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In the past decade, perovskite semiconductors have emerged as highly promising candidates for laser applications due to their desirable characteristics such as high mobility, modal gain coefficient, and oscillator strength [1]. Various forms of perovskites, including (quasi) two-dimensional, nanocrystals, and Dion-Jacobson have already demonstrated remarkable lasing properties [2]. While extensive research has been dedicated to optimizing device performance for perovskite solar cells and light-emitting diodes (LEDs), many existing reports predominantly focus only on demonstrating amplified spontaneous emission (ASE) or lasing, leaving a crucial gap in the development of a comprehensive strategy for reducing lasing thresholds and enhancing photo- and thermal-stability. Achieving population inversion in a perovskite gain medium necessitates a threshold carrier density of approximately  $\sim 10^{18} \text{ cm}^{-3}$ , which surpasses that required for LEDs by at least three orders of magnitude [3]. Consequently, the lasing operation within the perovskite layer results in the generation of substantial heat. In this study, we replaced the glass substrate with sapphire and employed graphite and copper as heat spreaders and sinks. Through this approach, we observed improved photo-stable ASE properties, particularly under intense excitation conditions. The guidance of lasing modes within the perovskite layer necessitates a minimum (cutoff) film thickness. Additionally, for better optical confinement, a thicker film is advantageous. Nevertheless, as perovskite is characterized by high absorption, excessively thick films result in elevated lasing or ASE thresholds. Consequently, an optimum film thickness exists to attain the lowest threshold. Here we conducted investigations to determine the optimal film thickness that demonstrates the lowest ASE threshold while maintaining a high output intensity.



**Figure 1 ASE Spectra under intense excitation for (a) glass/perovskite and (b) sapphire/perovskite/graphite/copper configurations. (c) Thickness dependence on ASE thresholds**

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# Elucidating Photostability of the Perovskite Films via Anti-Solvent Additive passivation

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In the recent decade, perovskite solar cells (PSCs) have emerged as a most promising photovoltaic technology because of their tunable band gaps, cost-effective manufacturing and improved performances [1]. Despite this, this technology has severe problems such as long-term stability, especially the photostability of these organic-inorganic PSCs, which restricting its commercialization. Moreover, these perovskite films are prone to heat, moisture and ultraviolet (UV) light causing decomposition [2,3]. Therefore, in this project, we introduced a highly efficient anti-solvent additive approach for the perovskite film passivation to overcome the photostability issues by incorporating various pyridine-based functional groups [4]. These functional groups possess a lone pair of electrons that can passivate into the perovskite film by ionic bonding with  $\text{Pb}^{2+}$ ,  $\text{I}^-$  to prevent decomposition [5]. With this, an enhanced device performance from 20.79 to 21.18%, and improved photostability, along-with reduced trap-density has been achieved

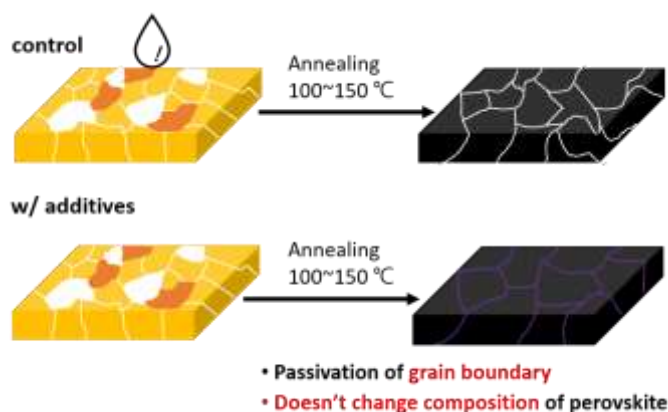


Figure 1 Schematic of the anti-solvent additive process.

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# Efficient all-thermally evaporated perovskite light emitting diodes for active matrix displays

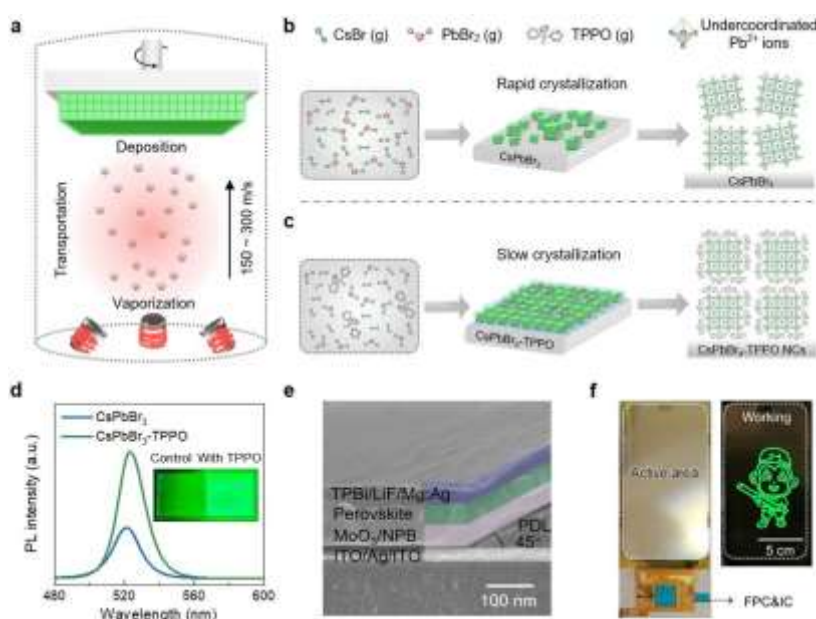
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Perovskite light-emitting diodes (PeLEDs) have recently demonstrated great potential for next-generation displays[1-3]. Fabricating PeLEDs by scalable and well-established thermal evaporation, the technique used for industrial manufacturing of organic LEDs, should accelerate the development of perovskite displays. However, the inferior device performance of thermally evaporated PeLEDs impedes their further display applications. The hidden reason is that the high energy states of thermally evaporated molecules contribute to the rapid crystallization kinetics of perovskite films, leading to massive defect states and disorder growth orientation. Here, we introduce Lewis base additives serving as surface passivator and crystallization retardant simultaneously during perovskite deposition, in-situ forming highly luminescent perovskite nanocrystals with suppressed defects and improved crystallinity. A peak external quantum efficiency of 16.4% is achieved for green PeLEDs with an all-thermally evaporated device architecture. We further fabricate active matrix PeLED (AMPeLED) displays by building them on conventional TFT substrates, which exhibit dynamic images with a resolution of 1080 × 2400. We anticipate that this work will stimulate the exploration of efficient vapor-deposited PeLEDs for industrial display applications.



**Figure 1 a**, Schematic diagram of tri-source thermal co-evaporation. **b, c**, Comparison of the crystallization process for thermally evaporated CsPbBr<sub>3</sub> and CsPbBr<sub>3</sub>-TPPO films. **d**, Photoluminescence spectra of CsPbBr<sub>3</sub> and CsPbBr<sub>3</sub>-TPPO films. **e**, Cross-section SEM image of the AMPeLED display panel, which shows one pixel. **f**, Photograph of the AMPeLED display panel.

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# Combinatorial slot-die coating of metal halide perovskite solar cells

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Metal-halide perovskite semiconductors are of interest for various optoelectronic devices: photovoltaics (PV), light-emitting diodes (LED), and photodetectors.<sup>[1]</sup> In order to accelerate the exploration of the compositional, structural, and opto-electronic properties of perovskite materials, we developed a high-throughput technique for the synthesis of thin film samples based on a two-ink differential feed using slot-die coating. As slot-die coating is a promising technique for solution processing of high-quality perovskite samples, this ensures that the described process can also be transferred for processing larger-area samples.<sup>[2]</sup>

As a first example, we use *combinatorial slot-die coating* to fabricate perovskite semiconductors of varying bandgaps by changing the ink ratio between two precursor inks of FAPbI<sub>3</sub> and MAPbBr<sub>3</sub>. We found that the coverage of high bromide samples resulted to be poor when fabricated under identical processing conditions optimized for iodide-based precursor inks, due to differences in the crystallization pathways of bromide and iodide-based perovskite.<sup>[3]</sup> This illustrates that there is a further need for the global optimization of both ink composition and process conditions to achieve the highest possible performance for all ink compositions. We further highlight our efforts to identify suitable processing conditions and gain insight into the formation mechanisms by using multi-modal analysis tools during slot-die coating. In solar cell devices, the composition of FA<sub>0.8</sub>MA<sub>0.2</sub>Pb(I<sub>0.8</sub>Br<sub>0.2</sub>)<sub>3</sub> yielded the best performance, which is consistent with the previously published result.<sup>[4]</sup> To characterize samples' micro- and macroscopic compositional homogeneity, we carried out morphological, optical, and crystallographic measurements on the samples.

The work presented is hence an example of how high-throughput strategies based on slot-die coating can be used to screen and explore the compositional and structural properties of metal halide perovskite semiconductors but also enable exploration of other solution-processable semiconductors in the future.

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# **In-situ analysis of solvent extraction process for large area perovskite film formation**

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Large area perovskite film deposition has been drawing considerable amount of interest to achieve the commercialization of perovskite during the past years. Differ from the conventional spin coating which normally adopts a dynamic antisolvent treatment to achieve high quality perovskite films, scale up methods require a different approach to achieve high quality films. Notoriously, dynamic antisolvent treatment for spin coating has a low reproducibility due to the manual errors such as antisolvent injection timing, injection rate, alignment, and height variations.

Here we report an antisolvent bath approach to achieve large area high quality perovskite films deposited via slot die coating with higher reproducibility. The as deposited film was placed into a customized quartz chamber filled with different antisolvent; a custom-made in-situ analysis equipment was used to monitor the photoluminescence (PL) and transmittance evolution of the perovskite film.

Several antisolvents with different miscibility to the host solvent (Dimethylformamide and Dimethyl sulfoxide) were chosen as the candidates. For PL analysis, peak intensity, peak position and peak full width at half maximum were tracked and analyzed. Diethyl ether (DE) showed better results with the highest peak intensity and slowest intensity increase rate.

In-situ transmittance analysis was also performed for the antisolvent stage as well as the thermal annealing stage using a pre-drilled hot plate kept at 100 °C. Transmittance at 480 nm and 750 nm were picked to track the evolution for antisolvent and annealing stages, respectively. Similarly, DE shows the slowest decay leading to uniform, dense film later confirmed by scanning electron microscope analysis.

Utilizing the results above, we applied a DE antisolvent treatment for slot die coated perovskite films. Devices were made from ITO substrate, SnO<sub>2</sub> (slot die coating), MAPbI<sub>3</sub> (slot die coating), Spiro-MeOTAD (spin coating) and gold (thermal evaporation). All coating procedures were carried out in ambient conditions. Champion device showed 18.57% efficiency with 23.48 mA/cm<sup>2</sup> short circuit current density, 1.06 V open circuit voltage and 0.75 fill factor. The antisolvent bath treatment proved successful for depositing large area high quality perovskite films. Coupled with in-situ analysis, it enables the precise pinpoint and manipulation of the processing window after the film deposition, which will be a huge benefit for industrial operations.

# Understanding the Space Charge Limited Current in Metal Halide Perovskite (SCLC)

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Metal halide perovskite semiconductors have sprung to the forefront of research into optoelectronic devices and materials, largely because of their remarkable photovoltaic efficiency records above 25% in single-junction devices and 28% in tandem solar cells, achieved within a decade of research [1]. Despite this rapid progress, ionic conduction within the semiconductor still puzzles the community and can have a significant impact on all metal halide perovskite-based optoelectronic devices because of its influence upon electronic and optoelectronic processes. This phenomenon thus also makes the interpretation of electrical characterization techniques, which probe the fundamental properties of these materials, delicate and complex. For example, space-charge limited current measurements are widely used to probe defect densities and carrier mobilities in perovskites [2]. However, the influence of mobile ions upon these measurements is significant but has yet to be considered [3,4]. Here we report the effect of mobile ions upon electronic conductivity during space-charge limited current measurements of MAPbBr<sub>3</sub> single crystals and show that conventional interpretations deliver erroneous results. We introduce a pulsed-voltage space-charge limited current procedure to achieve reproducible current-voltage characteristics without hysteresis.[5]

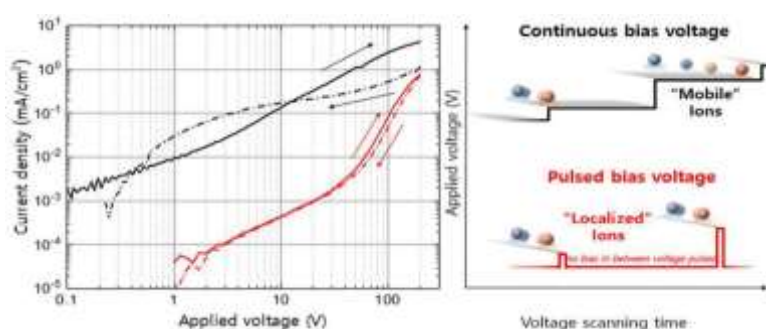


Figure 1 Schematic illustration of the principle and hysteresis in SCLC measurement.

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# Efficient HTL-free Perovskite Solar Cells via Surface P-type Doping

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Hole transport layer-free perovskite solar cells (HTL-free PSCs) have the advantages of simple device structure, low preparation cost and good stability, but the low photoelectric conversion efficiency hinders further development. The lack of hole selective extraction driving force at the perovskite/metal electrode interface results in serious interface recombination loss and limits device performance [1]. Based on the metal semiconductor contact theory, the surface p-type doping strategy was proposed, and the effect of this strategy in HTL-free PSCs was verified and optimized by wxAMPS software. After optimizing the perovskite layer thickness, surface doping depth, and defect density, the hole transport layer-free perovskite solar cell achieves a photoelectric conversion efficiency of more than 20%, which verifies the effectiveness of the surface p-type doping strategy. PEAI and F4TCNQ were used to modify the perovskite surface to passivate surface defects and achieve surface P-type doping, which increased the open circuit voltage and facilitated hole extraction, thus the champion HTL-free PSC obtained an open circuit voltage of 0.95V and achieved an efficiency of 14.86% [2].

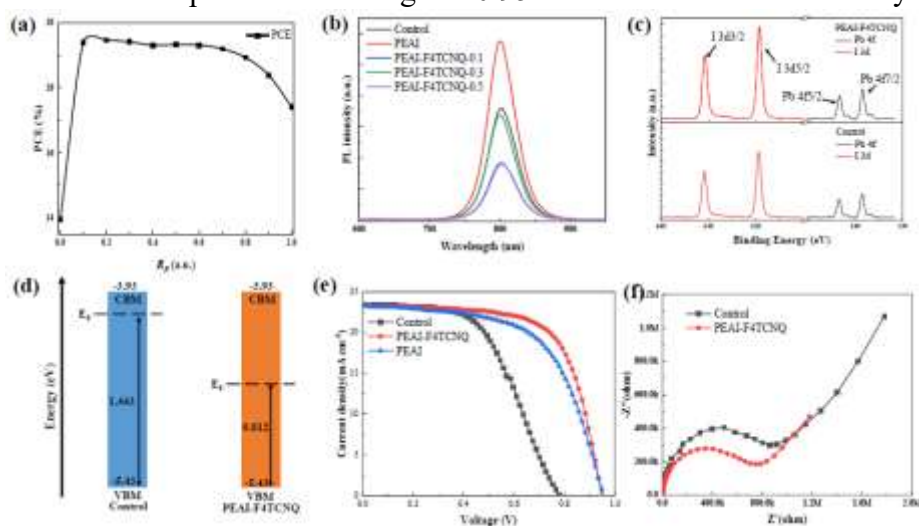


Figure 1 Surface P-type doping strategy improves the performance of HTL-free PSC. (a) Photoelectric conversion efficiency of the device under different P-type doping depth (RP) (b) Steady-state photoluminescence spectrum of perovskite film (c) XPS spectrum of I 3d and Pb 4f peak (d) Energy band diagram of perovskite film before and after modification (e) The JV curve of champion device (f) Electrochemical impedance spectroscopy

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# Exploiting the Synergies - p-i-n Carbon Perovskite Solar Cells with Fully Ambient Pressure Compatible Processes

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Record breaking lab scale PSC rely on evaporated noble metals as electrode materials. This is an expensive and slow process that impedes direct translation of the laboratory success of PSC into real world applications. A strong candidate to replace evaporated metal electrodes are carbon based materials deposited via solution process which promises cheaper, quicker to make, and more stable electrodes. Most publications on carbon electrodes for PSC are on devices in either the normal n-i-p or the hole transport layer free architecture. The transport layers used in n-i-p devices are however frequently linked to stability issues like the photoactive TiO<sub>2</sub> and SpiroOMeTAD which is frequently doped with hygroscopic salt. We have realised a solar cell in the more stable p-i-n architecture and without high vacuum processes via ambient carbon blade coating for the electrode. All layers in these devices are solution processed but an SnO<sub>2</sub> layer which is deposited by atomic layer deposition (ALD). ALD is quicker than evaporation and is compatible with higher throughput processes. This is the first reported p-i-n device without any evaporated layer and might pave the way to cheaper, industrial viable, and more stable PSC fully exploiting the synergies between carbon electrodes and the p-i-n structure.

# Two-Step Hybrid Perovskite Deposition: a Novel Crystal Engineering Approach and Vacuum-processed HTLs for Tandem Solar Cells.

Erica Magliano<sup>1</sup>

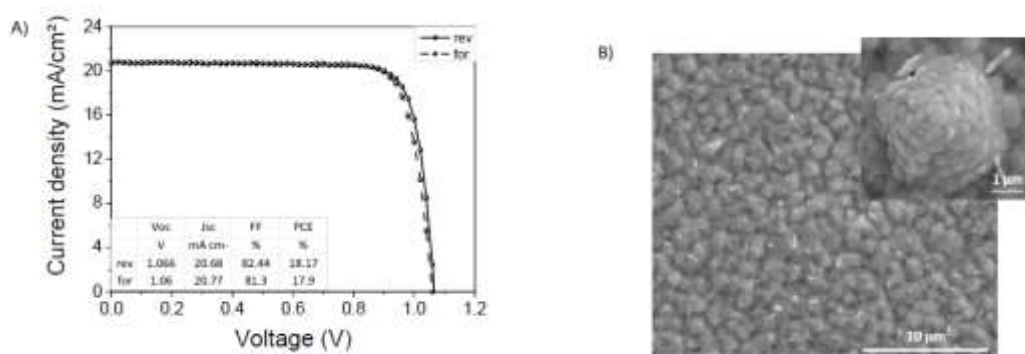
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Perovskite/silicon tandem solar cells represent the most straightforward solution to overcome single junction limit [1,2]. A conformal deposition of the perovskite top cell on silicon substrates represents a crucial aspect in monolithic tandem architecture. In this context, a two-step hybrid deposition (consisting of evaporation of the inorganic components and subsequent spin-coating of the organic salts solution) can ensure the advantages of vacuum deposition, such as conformability, while overcoming the drawbacks encountered in the evaporation of organic cations [3,4].

Here, a crystal engineering approach is followed to optimize the film morphology of two-step hybrid-deposited perovskite. The impact of different annealing conditions (such as humidity, solvents in atmosphere, sample coverage) on grain size, crystalline structure and device efficiency was investigated. The optimized final device had a power conversion efficiency (PCE) of 18.2% with a fill factor (FF) of 82.4% (Figure 1- A). With the final aim of fabricating monolithic perovskite/silicon tandem and to ensure a conformal coverage, vacuum-processed self-assembled monolayers (SAMs) were examined as hole transporting layers (HTLs). Evaporated MeO-2PACz showed the highest FF of 81.3%, whereas a superior  $V_{OC}$  of 1.07 V was measured on the evaporated Me-4PACz-based devices. The conformal coverage of the pyramids on textured silicon substrates of both HTL and perovskite was also successfully demonstrated (Figure 1-B). Thus, the present study paves the way for developing highly efficient tandem solar cells and the reported optimization can be applied to the perovskite top cell in monolithic tandem configuration.



**Figure 1: A) Current density-Voltage curve of the optimized two-step hybrid perovskite-based device; B) SEM images of two-step hybrid deposited perovskite on top of textured silicon.**

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# Mixed Monolayers as a Strategy to Improve the Performance of the Perovskite Solar Cells

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The use of phosphonic acid-based (self-assembled) monolayers has been rapidly expanding over the last several years. For the first time, carbazole-based materials 2PACz, MeO-2PACz, and Me-4PACz were used in CIGS/perovskite[1] and Si/perovskite[2] two-terminal tandem devices, leading to record efficiencies.

Due to the nature of the processing of the monolayers, there are several differences with the “traditional” bulk organic semiconductors. One of the examples is the straightforward way to use mixed monolayers. Simply mixing the two compounds in the precursor solution makes it possible to achieve the synergy between separate components.

Recently, an issue associated with poor wetting of Me-4PACz by perovskite precursor solution was resolved by utilization of the 1,6-hexylenediphosphonic acid as a second component.[3] Due to the presence of the polar groups at the surface of the monolayer, the contact angle between the substrate and solution decreased, resulting in effective coverage and a significant increase in the yield of the devices.

Small-area devices, fabricated with mixed monolayer kept a high performance of over 20% (demonstrated with “triple-cation” and “triple-halide” perovskite compositions). In addition, devices with an active area of 1 cm<sup>2</sup> were fabricated, with an average power conversion efficiency of 17.8% (18.7% best).

Following this example, further directions in the formation of mixed monolayers will be discussed in this presentation.

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[1] A. Al-Ashouri, E. Köhnen, B. Li, A. Magomedov et al. *Science* (2020), 370, 1300

[2] A. Author, B. Author and C. Author, *Journal* (Year), Volume, pages. A. Al-Ashouri, A. Magomedov, M. Roß et al. *Energy Environ. Sci.* (2019), 12, 3356-3369

[3] A. Author, B. Author and C. Author, *Journal* (Year), Volume, pages. A. Al-Ashouri, M. Marčinskas, E. Kasparavičius et al. *ACS Energy Lett.* (2023), 8, 898

# Novel low-temperature laminable encapsulants based on two- dimensional hexagonal boron nitride for perovskite solar cells and modules

Paolo Mariani<sup>1</sup>

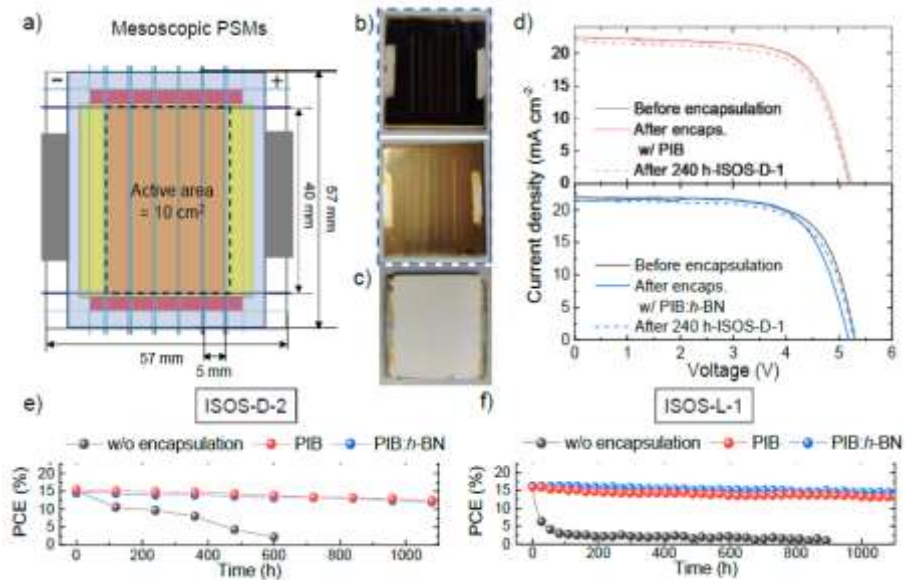
Miguel Molina,<sup>2</sup> Marilena Isabella Zappia,<sup>2</sup> Erica Magliano,<sup>1</sup> Luigi Angelo Castriotta,<sup>1</sup> Francesco Di Giacomo,<sup>1</sup> Luca Gabatell,<sup>2</sup> Sebastiano Bellani,<sup>2</sup> Aldo Di Carlo,<sup>1</sup> Francesco Bonaccorso<sup>2</sup>

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Perovskite solar cell (PSC) technology has currently reached a certified power conversion efficiency (PCE) above 25% [1]. This outstanding PCE has been achieved using direct (n-i-p) cell structures [2], which are the most reliable ones in terms of both photovoltaic performances and validated into large-area formats (including the first PSC solar farm [3]). Nevertheless, PSCs' stability must be still improved to meet the targets required for widespread market (> 10+ year lifetime)[4]. To this end, advanced encapsulants compatible with thermal and chemical stability of perovskites are needed to stabilize the PSC performances, during prototypical accelerated life tests, including ISOS and IEC ones.[5] In this work, we report a successful low-cost encapsulant/glass stack encapsulation approach for both PSCs (cells) and PSMs (modules), i.e. the blanket-cover approach. The encapsulant consists of viscoelastic polymeric composite incorporating two-dimensional (2D) flakes of hexagonal boron nitride (h-BN). The latter, produced at industrial scale through wet-jet milling exfoliation [6], act as physical barriers against environmental agents, including oxygen and moisture, improving the overall barrier properties of the pristine PIB (polyisobutylene) encapsulant along its mechanical and thermal management characteristics. The encapsulation process was carried out at low temperature (between 60 °C and 90 °C) using an industrial laminator. Water Vapor Transmission Rate (WVTR) of our encapsulating stack results as low as  $\sim 10^{-5} \text{ g m}^{-2} \text{ day}^{-1}$ . [7] Without any edge sealant, our encapsulated PSCs and PSMs based on  $\text{Cs}_{0.08}\text{FA}_{0.80}\text{MA}_{0.12}\text{Pb}(\text{I}_{0.88}\text{Br}_{0.12})_3$  withstood multifaceted accelerated aging tests, including ISOS-D1 (shelf life storage under ambient conditions), ISOS-D2 (damp heat, >1000 h), ISOS-L1 (light soaking, >1000 h), as well as customized thermal shock (200 cycles with abrupt temperature changes between +85 and -20 °C) and humidity freeze (10 cycles with abrupt temperature changes between +85 and -20 °C and including a water immersion step before device freezing) tests, retaining more than 80% of their initial (at the beginning of the test) power conversion efficiency (PCE). Our work shed light on the use of advanced low-temperature encapsulants for the massive fabrication of stable perovskite-based photovoltaics, including, beyond PSCs, next-generation perovskite-based tandem systems.



**Fig. 1. a)** Schematic of the mesoscopic PSM layout (cell active area = 2 cm<sup>2</sup>; total active area = 10 cm<sup>2</sup>), in which the non-compact layers of the device are totally covered by the encapsulant. **b)** Photograph of a representative mesoscopic PSMs, as fabricated (front and rear sides: top and bottom picture, respectively) and **c)** after encapsulation (rear side) with PIB:h-BN. **d)** JV curves (reverse voltage scan) measured for the as-fabricated mesoscopic PSMs before and after encapsulation with PIB (top panel) and PIB:h-BN (bottom panel) (before and after 240 h-ISOS-D-1). **e, f)** PCE trend of the PSMs without encapsulation and with PIB and PIB:h-BN encapsulants acquired over >1000 h of the ISOS-D-2 and ISOS-L-1 tests

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# Single crystal 2D perovskite thin films for solar cells

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2D Ruddlesden-Popper perovskite phases in solar cells have been exploited in combination with polycrystalline (PC) 3D HPs as ultrathin passivation layers to improve stability and charge extraction. Most of 3D/2D heterostructures reported so far are made by PC thin films grown on top of PC 3D HPs, with little control over orientation and crystalline phase, thus creating high concentration of defects at grain boundaries and interfaces, which favors the presence of traps for charge carriers, ion migration and water permeation.

On the other hand, pure 2D HPs in solar cells have been considered less suitable for photovoltaics due to their large exciton binding energies which should hinder charge separation by a significant energy loss. Surprisingly, the presence of large polarons, that is charge carriers coupled to lattice deformations, inhibits the formation of excitons and appears to be the microscopic mechanism enabling efficient 2D HPs solar cells[1,2].

The use of single crystal (SC) HPs both for 2D/3D heterostructures and pure 2D film devices is still challenging and their performance is even lower than PC devices due to the high density of traps at the crystal surface.

Here we explore single crystal perovskite 2D/3D heterostructures and pure 2D layers. Growth of 2D HPs single crystal thin films is shown for several organic molecules and their optical and structural properties are studied. Single crystal 2D/3D thin film heterostructures are also shown and various strategies for interface engineering are proposed. We finally present a critical comparison of the photophysics of single crystal and polycrystalline devices.

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[2]Simbula et al. <https://doi.org/10.21203/rs.3.rs-2378521/v1A>.

# 2D layered hybrid perovskites featuring benzotriazole-based organic cations: a fundamental study of structural and optical properties

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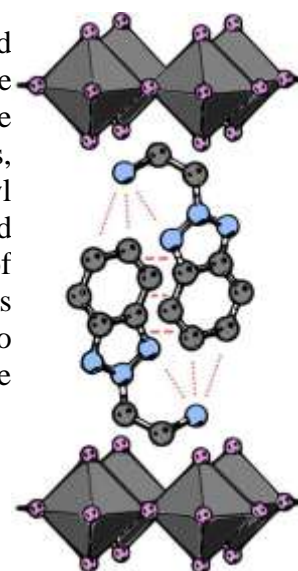
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2D layered hybrid perovskites are currently being investigated as an alternative to 3D hybrid perovskites, which suffer from limited stability against moisture, prolonged illumination, and temperature. In state-of-the-art 2D layered perovskites, butylammonium (BA) and phenethylammonium (PEA) cations are still mostly employed. Although these organic cations succeed in stabilizing the perovskite, they don't offer valuable properties of their own to complement the attractive optoelectronic properties of the perovskite layers. Synergy could be achieved by choosing larger organic cations with more suitable opto-electronic properties [1,2], or by inserting organic charge-transfer complexes [3] or dipole stacks in the organic layers.

In this work, benzotriazole-based organic cations are synthesized and subsequently successfully applied to 2D layered hybrid perovskites. The structural and optical properties of thin films and single crystals of these perovskites are investigated. We show that the synthesis of these cations, films, and crystals is straightforward and that the aromatic substituents and the alkyl tail length can be readily varied. The tendency to form dipole stacks and intermolecular and intramolecular hydrogen bonds, combined with the ease of substituent implementation, render benzotriazole-based perovskites susceptible to organic layer engineering in a more advanced way compared to BA-based and PEA-based perovskites. This could ultimately improve the performance of 2D layered perovskites in various applications.



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# Dipole modification of the perovskite/C<sub>60</sub> interface upon piperazinium iodide treatment - a Near-UV photoemission spectroscopy study

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In recent high efficiency silicon/perovskite tandem solar cells, C<sub>60</sub> is most widely used as electron-selective contact. This interface is however known to limit the open-circuit voltage ( $V_{oc}$ ) of the devices, which might be caused by non-radiative recombination, an unfavourable conduction band offset at the interface, or a combination thereof [1]. In a previous study, we find a large energetic offset between the perovskite conduction band minimum (CBM) and the C<sub>60</sub> lowest unoccupied molecular orbital (LUMO) which contributes to the limitation of the  $V_{oc}$  [2]. To omit these losses different interface modifications such as LiF [3] or piperazinium iodide (PI) [4] are explored, leading to remarkably high  $V_{oc}$ s in our current world-record perovskite/silicon tandem solar cells with 32.5% power conversion efficiency.

In this contribution, we apply a rarely used photoemission yield spectroscopy technique with near-UV excitation in constant final state mode (CFSYS) on device-relevant samples. This method enables to i) probe directly the characteristically low density of states at the valence band maximum (VBM) of the perovskite, including defect states within the band gap, and ii) observe the perovskite VBM below thin layers of C<sub>60</sub> to directly access the energetics at the interface with an enhanced information depth as compared to standard methods. We find that PI induces a dipole of around 350 meV (Figure 1), reducing the CBM-to-LUMO offset to almost 0 eV and thereby leading to a favourable band alignment that enables high  $V_{oc}$ s in full devices.

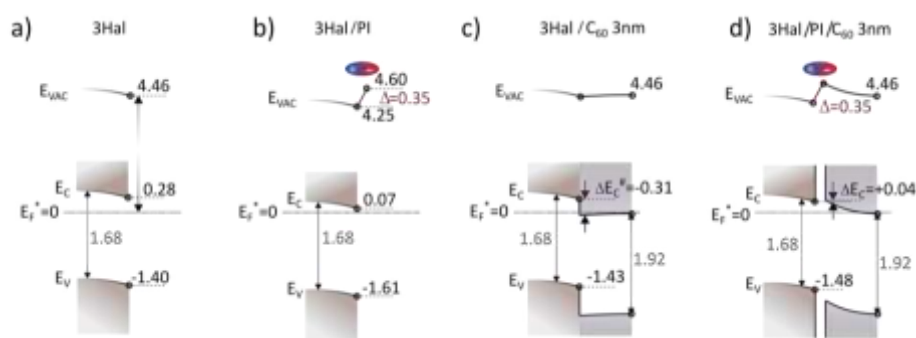


Figure 1: Band alignment of the PI-modified triple halide perovskite/C<sub>60</sub> interface

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# Origin of the Voc growth in perovskite solar cell with Br substitution

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Metal halide perovskite has emerged as the promising photovoltaic material during the last decade. Particularly, most high performance perovskite solar cells are based on mixed iodide-bromide halide perovskite.[1] However, the understanding of the Br substitution on device performances is still unclear. Here, we attempt to introduce 5% Br into MA based perovskite to compare its device performance with the perovskite without Br. We observed that the open circuit voltage was enhanced (Figure 1), and the crystallinity of the perovskite is better. In addition, with the Br substitution, it was observed by GIXRD that the strain inside perovskite is released. Moreover, to bridge the gap between materials properties and the charge dynamics in devices, we also used a series of novel pump-push-photocurrent spectroscopy (PPPC) to investigate the charge recombination mechanism and trap density in perovskite solar cell. From these results we gain some insights that Br substitution is a promising way to manage the traps distribution in perovskite to boost the device performances.

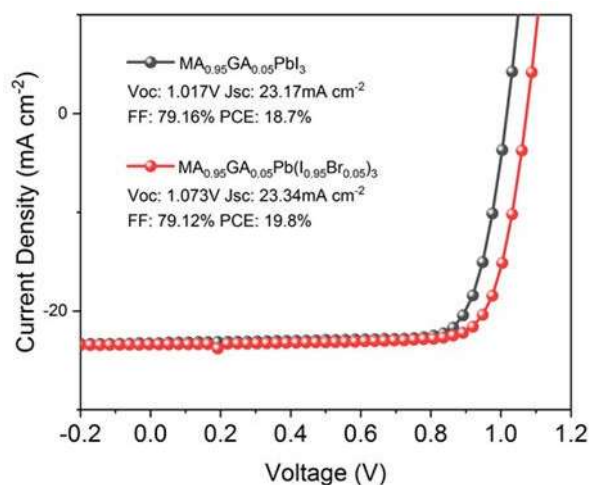


Figure 1 J-V curves of the inverted perovskite solar cell with and without Br.

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# Two-step evaporation of low-bandgap mixed lead-tin perovskites for solar cells

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All-perovskite multi-junction perovskite solar cells (PSCs) are an exciting opportunity for next-generation solar cells [1]. Vapour deposition processes present a solvent-free fabrication route, suitable for depositing perovskite materials on stacked layers and on large-area substrates, rendering this technique ideal for large-scale manufacturing of multi-junction PSCs [2]. To date, evaporation of wide-bandgap (1.5 - 1.8 eV) perovskite materials has been achieved [3,4]; however, low-bandgap PbSn materials are yet to reach the same level of success [5]. The progress in the area of PbSn evaporation has been more limited than for the wide-bandgap materials, since it is preferred to have a separate evaporator used solely for Sn-based materials to avoid cross-contamination, and current efforts have focused on single-step co-evaporation [5,6]. Here, we report the fabrication of  $\text{FA}_{1-x}\text{Cs}_x\text{Pb}_{0.5}\text{Sn}_{0.5}\text{I}_3$  via a two-step evaporation process. In this process, an inorganic layer is deposited via co-evaporation before an organic layer is deposited. We observe conversion of the two layers into a perovskite structure after a thermal annealing step, and the structural and optoelectronic properties of the resulting perovskite film are characterised.

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# Multifunctional Leek-Inspired Light Management Layer for improving the performance of perovskite solar cells

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This study introduces a facile approach to enhance the performance of perovskite solar cells (PSCs) through the integration of light management layers (LML) [1]. The proposed LML consists of cellulose acetate films patterned by replicating the surface structure of common leek leaves. In addition to high transparency at visible wavelengths, the resulting films possess haze and self-cleaning properties. Implementing the hazy LML onto triple cation PSC devices, illustrated in Figure 1, improved the power conversion efficiency, with a measured increase of  $6\pm 0.3\%$ . Furthermore, by adding Carnuba wax (CW) the films' surface water repellence significantly increased which could enable self-cleaning, effectively addressing dirt accumulation. Moreover, the CW-treated films offer UV absorbance which leads to incident light screening and ensures sustained and durable photovoltaic performance.<sup>[2]</sup>

In particular, the replication method employed in this research illustrates the potential of using naturally patterned surfaces as templates for fabricating substrates. Looking ahead, employing biobased materials as PSC substrates can offer improved sustainability and easy recycling of these devices. Ultimately, this study paves the way for more efficient and environmentally friendly PSCs in the field of renewable energy.

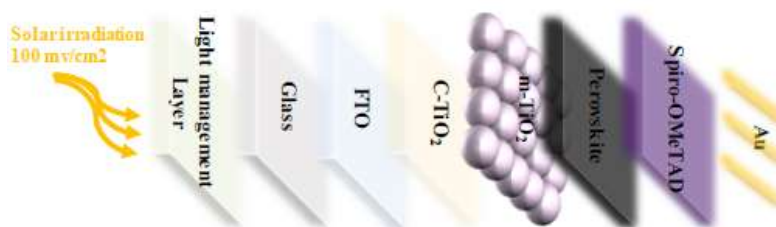


Figure 1 Schematic of LML integrated perovskite solar cells.

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# Unrevealing Defects during Lead-Halide Perovskite Film Formation

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Lead-halide perovskites have established a firm foothold in photovoltaics and optoelectronics due to their steadily increasing power conversion efficiencies approaching conventional inorganic single-crystal semiconductors.<sup>1,2</sup> However, further performance improvement requires reducing defect-assisted, nonradiative recombination of charge carriers in the perovskite layers.<sup>3</sup> A deeper understanding of perovskite formation and associated process control is a prerequisite for effective defect reduction.

In this talk, a combination of techniques will be presented, including in-situ photoluminescence (PL) spectroscopy and grazing-incidence small/wide-angle X-ray scattering (GI-WAXS/SAXS), to study the structural and optoelectronic kinetics during MAPbI<sub>3</sub> and FAMAPbI<sub>3</sub> perovskite formation. The growth kinetics were studied for vapor-deposited perovskites, as well as for perovskite layers fabricated from the wet phase. The results reveal the formation of MAPbI<sub>3</sub>-based perovskites from the early stages and uncover the morphology, crystallographic structure, defect density, and strain evolution. We observed that the growth of perovskite nanocrystals is manifested in rapid PL intensity increase and a substantial PL redshift. Furthermore, the overall nonmonotonous character of PL intensity during the perovskite formation reflects the perovskite phase volume and the defects states at the perovskite layer surface and grain boundaries. Interestingly, the PL intensity evolution is similar for both – liquid-based and vapor-based perovskite fabrication techniques. Such observation indicates an analogous mechanism of defect development despite different chemical processes taking place during perovskite formation. Besides, the crystallographic analysis performed by GIWAXS revealed the strain transformation from compressive to tensile upon coalescence of individual perovskite grains.

**Acknowledgment:** *This work was supported by APVV-21-0297, SK-CZ-RD-21-0043, SK-AT-20-0006, BMBF and DFG, and ITMS 313021T081.*

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# Scalable Fabrication of Pure Formamidinium based Perovskite Solar Cells by Slot- Die Coating Process

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The halide perovskites (HPs) have recognized in the field of photovoltaics (PVs) that accredited from their remarkable optoelectronic properties and are capable to compete in terms of power conversion efficiencies (PCE) with the traditional contenders like silicon, gallium-arsenide based solar cells, etc. Towards the commercialization goals and the “lab to fab” concept for the PV based devices from HPs, there are numerous stringent norms that must be satisfied in terms of long-term device stability, perovskite material stability, and facile fabrication procedures, etc.

Though, majority of the high-efficiency solar cells are mostly fabricated under a controlled and an inert environment with a small area (less than 1 cm<sup>2</sup>) devices, and which are unfeasible for the large-area/module device (area greater than or equal to 800 cm<sup>2</sup>) fabrication and cost effectiveness.[1,2,3] Hence, it is mandatory to have a relatively low-cost fabrication processes which are key requirements for the large scale and commercialization goals. In addition, not only the high efficiency standards have to be fulfilled but also the photoactive perovskite phase should be inherently stable towards several stringent situations to ensure the long-term stability of the efficient and working PV devices.[3]

The formamidinium lead iodide (FAPbI<sub>3</sub>) is showing the lowest bandgap (1.48 eV) value among the group of lead-based HPs and promised to have a maximum Shockley-Queisser (SQ) theoretical efficiency of ~33%.[2,3] Though, the thermodynamically triggered polymorphism behaviour and the presence of non- photoactive phase curtail the potentiality of this HPs in efficient and stable optoelectronic devices. Therefore, the FAPbI<sub>3</sub> phase stabilization without any significant bandgap blue-shifting materials that are highly demanded for the large area PV devices. Here, we demonstrated the slot-die ink tailoring with the cumulative effect of solvents and additives for the formation of smooth and defect free FAPbI<sub>3</sub> perovskite thin films. The well optimized FAPbI<sub>3</sub> perovskite thin film demonstrated with > 21% (for small area of 0.09 cm<sup>2</sup>) and 16% (for laser series interconnected modules of 9 cm<sup>2</sup>) of PCEs. These findings focus the great promise of scalable slot-die techniques in the growth of stable and high-quality FAPbI<sub>3</sub> perovskite thin films for PV technologies.

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# Defect tolerance and improved stability in 1.8 eV bandgap perovskite solar cells activated by Ionic Liquid Passivation

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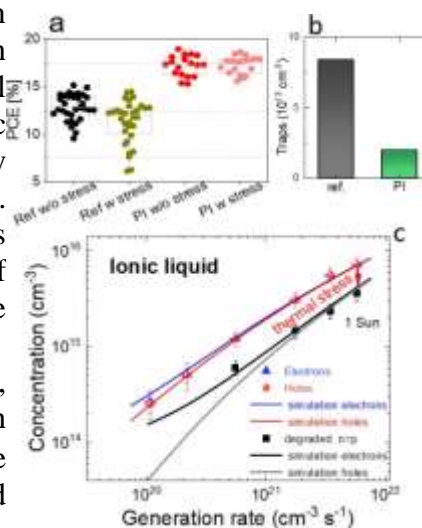
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Low-cost metal halide perovskite semiconductors (MHP) can potentially provide a significant boost in solar cell conversion efficiency through versatile and easy-to-control electrical structure, morphology, composition, and optoelectronic properties[1]. Various strategies were used to improve the stability and efficiency of PSCs, including additives and passivation layers. However, the unsatisfied stability of perovskite still constrains further development for the final commercialization. Passivation of surface defects showed a significant influence on the HPS charge transport properties and stability[2].

Li *et al.* demonstrated the novel bifunctional ionic liquid, piperazinium iodide (PI), the molecule of which contains both positive ( $R_2NH_2^+$  electron acceptor) and negative. We demonstrate that PI-treated PSCs maintain almost unchanged efficiency after 18 hours of thermal stress at 85 °C, as demonstrated in Fig. 1a. We show the change in the crystal structure, optoelectronic, charge transport and material properties of perovskite before and after thermal stress (Fig 1b). We implicate for the first time the Constant Light Induced MAGneto Transport to demonstrate the effect of degradation on steady-state carriers' concentration, lifetime, and diffusion length, at the condition close to the solar cells' operation at one sun illumination, as demonstrated in (Fig 1c).. The experimental results are further supported by theoretical charge transport simulation, which discloses the formation of additional electronically deep defects in degraded perovskite material (Fig 1b). As a conclusion of the deep fundamental and applied study, we demonstrate that implication PI ionic liquid passivation leads to defects suppression in halide perovskite even under thermal stress resulting in higher operational stability of solar cell devices. Therefore, our findings reveal a new approach to trigger and tackle defect tolerance in photovoltaic materials.



**Figure 1. a, Performance of PSCs before and after thermal stress. b, Concentration of defects in ref. and PI treated halide perovskite after thermal stress, and c, Example of constant light induced magneto transport measurements probed before and after thermal stress in MHP treated by PI**

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# Thermal disorder-induced carrier localisation activates reverse halide segregation.

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Inhomogeneity of the bandgap due to photo-induced halide segregation is challenging the prospect of commercialization. While the reversal of halide ions has been studied under various conditions, the underlying mechanism of heat-induced reversal remains unclear. In this work, it is shown that disorder-induced localisation of self-trapped polarons reverses segregation. Localization of polarons is observed to result in one order magnitude decrease in excess carrier density (polaron population) resulting in a reduced impact of the light-induced strain (LIS) on the perovskite lattice (responsible for segregation). An interplay between the enthalpy of segregation and entropy of remixing could be regarded as an interplay between driving forces, LIS and thermal disorder-induced strain (TDIS). Upon in-situ heating of a wide-bandgap perovskite thin film to 80 °C under continuous 0.1 W/cm<sup>2</sup> illumination (upon reversal of segregation), the lattice strain disorder increased by ~77% with a corresponding increase in lattice parameters. Meanwhile, TDIS at 80 °C under dark conditions (0.23%) exceeded the value imposed by 1-Sun illumination intensity (0.14%). Therefore, exposing the lattice to larger global strain could eliminate photoexcitation-induced strain gradient, as thermal disorder causes a reduction in excess carrier density, and the effect of the LIS strain could be masked by thermal fluctuations of the lattice. The results are further supported by various temperature-dependent in-situ measurements as well as simulations. These findings highlight the importance of strain homogenization and indicate a potential pathway for designing optimally strained, stable perovskites for real-world operating conditions.



# Unveiling the translational impact of electron transport layers on perovskite film formation.

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All-inorganic absorbers are a growing area of interest within perovskite photovoltaics, by combining the ever-increasing efficiencies of perovskite solar cells with less air-sensitive, more temperature-stable materials – removing the issues of instability in mixed halide perovskites [1]. A particularly promising candidate within this area is CsPbI<sub>2</sub>Br, with a low-annealing temperature, and efficiencies now exceeding 17% [2]. Much focus is paid to improving the morphology of the perovskite material through doping [3,4], post-treatments [5,6], all with the aim of passivating defects, improving interfaces and improving efficiency.

The role of electron transport layer (ETL) is also a vital factor when manufacturing the perovskite solar cell, with TiO<sub>2</sub>, SnO<sub>2</sub> and ZnO all being popular choices [7-9]. As the push towards higher efficiencies and commercialisation proceeds, there is a desire to ensure that the process of manufacture is cost-effective, and does not contain high-temperature annealing steps, currently widely used in TiO<sub>2</sub> deposition.

Whilst attention is paid to the extraction capability of the electron transport layer, and additives are explored to enhance the interface [10], little attention is played to the role that the electron transport layer on crystallisation of the perovskite. In this present work, electron backscatter diffraction (EBSD) mapping, x-ray diffraction (XRD) and cathodoluminescence (CL) hyperspectral imaging are utilised to reveal how ETL layer dictates the crystallographic and optoelectronic properties the perovskite film. EBSD is used to show how the grain size and orientation in the perovskite films is impacted by electron transport layer, when the absorber is grown at different temperatures, whilst cathodoluminescence shows unexpected heterogeneity in the films, with wavelength shift of emission between samples. XRD confirms that the phenomena observed in the EBSD measurements are consistent across the entire sample size. This work gives a new insight into the role of the ETL on perovskite growth, and why selection of this layer must be justified.

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# Strategy for in-air deposition of perovskite cell and modules: Comparison between TiO<sub>2</sub> and SnO<sub>2</sub> transporting layers

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In recent years, perovskite solar cells have (PSCs) captivated attention due to their potential superior properties compared to silicon solar cells [1-3]. Despite the remarkable efficiencies reported for lab-scale PSCs, achieving large-scale devices without remarkable efficiency loss in pilot line remains challenging [4]. Scalable deposition methods are necessary for commercializing PSCs, but upscaling to large area module level devices and addressing reproducibility issues remain a struggle [5-7]. In this work, we compare TiO<sub>2</sub> (mesoscopic structure) and SnO<sub>2</sub> (planar) ETL (electron transport layer) layers by adopting semi-automatic deposition techniques as spray- and blade-/slot-die coating in ambient air. The perovskite precursor solution was deposited by semiautomated scalable process in ambient air based on blade coating technique in n-i-p configuration. The experiment evaluates homogeneity of meniscus-based and liquid spray deposition techniques on a 32 cm<sup>2</sup> glass substrate compared to spin-coating, and highlights performance, morphology and thickness variations across different module regions. The automated deposition offers a scalable method for several large area cells on a module substrate achieving a power conversion efficiency up to 18% with high reproducibility. We up scaled the results to a mini-module with a size of 32 cm<sup>2</sup>. Various characterization techniques including SEM, profilometer, UV-vis, and PL spectroscopy are employed to evaluate the properties and uniformity of the film deposition. The obtained results indicated that spray automated method can provide scalable and reliable technology for fast and efficient mesoporous deposition.



**Figure 1 Automated spray coating for TiO<sub>2</sub> mesoporous for modules**

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# N-Octylammonium Bis(trifluoromethylsulfonyl)imide as a Highly Functional Additive for Spiro-OMeTAD Layer in Perovskite Solar Cells

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Room-temperature ionic liquids (RTILs) are promising additives for hole transport materials (HTMs) in perovskite solar cells (PSCs) as it does not require lithium (Li) species, which is likely detrimental to the photovoltaic performances, and can provide additional benefits. However, design of RTILs for the PSC application have been limited so far within the currently major components such as bulky quaternary ammonium-, pyridine-, and imidazole-based cations, which has confined their functions.

Herein, an RTIL comprising aliphatic primary ammonium (i.e., *n*-octylammonium: OA) cations, which is the archetype RTIL cation found over a century ago (Figure 1), and modern bis(trifluoromethylsulfonyl)imide (TFSI) anions [1,2] is proposed and demonstrated as a preferable additive for Spiro-OMeTAD HTM in PSCs. The OA cations spontaneously and densely passivate the perovskite layer during the HTM deposition process, leading to both suppression of carrier recombination at the HTM/perovskite interface and hydrophobic perovskite surfaces. Meanwhile, the TFSI anions effectively improve the HTM function most likely via efficient stabilization of Spiro-OMeTAD radical, enhancing hole collection properties in the PSCs. Consequently, PSC performances involving the long-term stability were significantly improved using OA-TFSI additive.

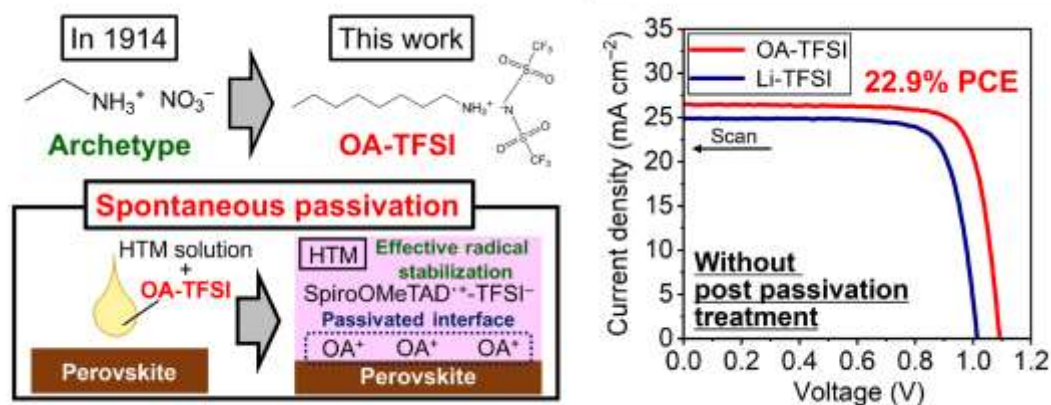


Figure 1. Conceptual schemes of spontaneous passivation by OA-TFSI and J-V curves of PSCs with additives of conventional Li-TFSI or OA-TFSI in this work

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# CsPbI<sub>3</sub> towards Tandem application

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We demonstrate a simple approach for a stable CsPbI<sub>3</sub> in environmental condition, retaining its black phase in air for a week, without encapsulation. We also demonstrate the feasibility of semi-transparent devices suitable for silicon coupling. The NIP device stack is as follows: glass-FTO/cTiO<sub>2</sub>/SnO<sub>2</sub>/PSK/Passivation layer/PTAA/Ag or ITO. 0.6 M CsPbI<sub>3</sub> perovskite solution is fabricated from CsI, PbI<sub>2</sub>, and DMAI precursors with a molar ratio of 1:1:1.5 and dissolved in DMF. DMAI will form an intermediate DMAPbI<sub>3</sub> with PbI<sub>2</sub>, then, DMA will sublime during the annealing process letting Cs<sup>+</sup> cation take its place in the crystal lattice [1], leading to a fully inorganic absorber. Perovskite is deposited on cold substrates and annealed at 100 °C for 10' and then at 200 °C for 2', to complete the phase conversion. Then, samples are put at room temperature to block the black phase with a thermal shock [2]. A PMMA (0.4 mg/mL in CB) passivation layer is spin coated on top of the perovskite, to insulate the absorber layer while still ensuring a good charge extraction thanks to the low concentration [3]. Both thermally evaporated Ag contacts (0.2 cm<sup>2</sup>) and sputtered ITO (0.4 cm<sup>2</sup>) are used to finalize the devices, obtaining an enhanced black phase retention in environmental conditions for more than one week without any encapsulation.

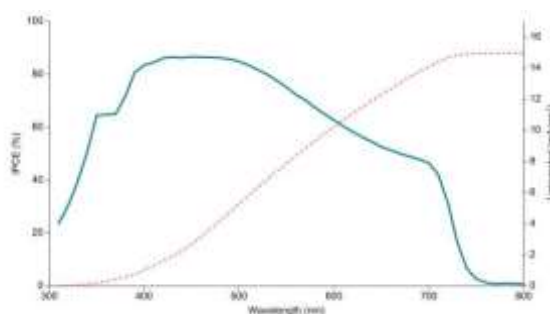


Figure 1 IPCE of CsPbI<sub>3</sub> device with ITO semi-transparent electrode.

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# Flash Annealed Nickel Oxide for Large Area Perovskite Solar Cells

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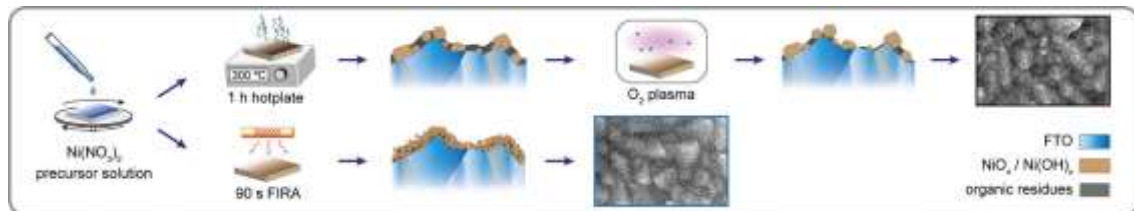
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Stability and scalability remain the two most urgent challenges preventing the mass deployment of Perovskite solar cells (PSCs). The highest efficiency PSCs reported use proprietary organic hole transport layers (HTL) such as Spiro-OMeTAD, PTAA or the novel carbazole-based self-assembled monolayers (SAMs). These materials require long annealing or synthesis protocols, in other occasions, repeated washing steps are necessary diminishing their industrial and environmental appealing.

Non-stoichiometric nickel oxide ( $\text{NiO}_x$ ) is an inorganic p-type semiconductor, it is an earth abundant material and its low cost and stability make it a strong candidate for industrial production of devices.  $\text{NiO}_x$  is deposited mostly through sputtering or solution processing, requiring the use of high vacuum or long and costly synthesis or post- treatments. On the contrary, Flash-Infrared-Annealing (FIRA) provides a fast and localized temperature increase of the substrate surface, reducing the processing time to the order of seconds.



**Figure 1 Example of a figure caption. Use 10 point Times New Roman.**

The use of FIRA allowed to produce  $\text{NiO}_x$  in atmospheric conditions, reducing the sintering time by 97%. In this work, we consider a line shape model to analyse the Ni 2p spectrum and quantify the composition of the  $\text{NiO}_x$  films and their stoichiometry. The results indicate that the presence of  $\text{Ni(OH)}_2$  residues can cause a potential lifetime reduction in p-i-n devices. Compared to traditional annealing methods, FIRA results in a more complete conversion to  $\text{NiO}_x$  with lower concentration of  $\text{Ni(OH)}_2$  residues and higher oxygen-to-nickel ratio. An efficiency of 16.7% was obtained for planar and inverted PSCs of  $1 \text{ cm}^2$  and 15.9% averaged over an area of  $17 \text{ cm}^2$ , while at the same time increasing the stability by 36%.

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# Polarimetric measurements of the bright triplet emission of single cesium lead halide perovskite quantum dots at cryogenic temperature

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Cesium lead halide perovskite quantum dots (QDs) have recently emerged as promising platform for quantum light sources. Indeed, they exhibit exceptional photoluminescence properties thanks to the emission from a bright triplet exciton state [1]. The energetic fine structure splitting, in the order of a few millielectronvolts, can be revealed by performing single QD spectroscopy at cryogenic temperature. In particular, depending on the QD orientation and on the observation direction, up to three orthogonal emitting dipoles can be spectrally detected, each of them with a high degree of linear polarization. To measure the polarization of the exciton fine structure, typically a rotating linear polarizer was used. However, this method cannot provide a complete characterization of the polarization state of the emitted light, and the polarization properties of the small, non-linearly polarized fraction of the emission were unclear.

That is why in this work we are investigating the polarization properties of individual cesium lead halide perovskite QDs by more advanced polarimetric techniques that allow to measure the complete Stokes polarization vector at cryogenic temperature for each emission line. For these measurements it is crucial to perform a careful calibration of the optical path with respect to residual, unwanted birefringent phase shifts that are often occurring from optical coatings. Moreover, these measurements require colloidal QDs with very low intermittent emission fluctuations. In my presentation I will report the results of the polarimetry of single perovskite QDs, shedding light on the non-linearly polarized emission fraction and the nature of their peculiar emission properties.

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# Fundamental analysis of all inorganic germanium perovskite

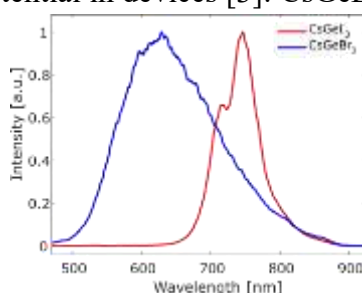
Andrea Olivati<sup>1,2</sup>

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In the last years a great interest has been spent in study lead-free perovskite, in particular one of the first investigated alternative to lead for optoelectronic application was Germanium [1, 2]. Despite the early interest there is still a leakage of knowledge about the fundamental optical properties of this class of materials. Among this huge family we choose to focus on two completely inorganic germanium perovskite due to their promising potential in devices [3]: CsGeBr<sub>3</sub> and CsGeI<sub>3</sub>.



**Figure 1** Photoluminescence of CsGeBr<sub>3</sub> and CsGeI<sub>3</sub> under pulsed excitation (355 and 532 nm respectively) at room temperature.

The first sample shows a very broadband emission centered at 640nm at room temperature and an excitonic peak appears lowering the temperature. To understand the nature of this broadband emission we performed an in depth structural and optical analysis and we can address it to defect assisted or Self-Trapped excitons recombination.

The second investigated perovskite shows a featured emission centered at 740nm. Lowering the temperature and increasing the incident light intensity a very sharp peak associable with ASE appears. To address the origin of this featured peak we performed time, temperature and fluence dependent photoluminescence measures.

We think that this work can give some insight in the fundamental properties of this class of material which is worthy of further studies.

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# Lead-free Magnetic Halide Perovskite Photovoltaics

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Over the recent years, seminal contributions to non-magnetic Hybrid organic-inorganic lead halide perovskites (MAPbX<sub>3</sub>) have been underpinned by several viable strategies with a view to tackle critical challenges involving photoconversion efficiency (PCE), instability, and lead toxicity. An aspect that remains underexplored but presents a lot of promise is the magnetic spin degrees of freedom available in magnetic perovskites to tune the photovoltaic (PV) properties, which in all likelihood can lead to staggering spin related properties[1]. The interplay of two spin degrees of freedom in these magnetic systems gives a wider platform for modulating the absorption range with an attempt to harvest the entire solar radiation spectrum.

Herein, we report the magneto-optoelectronic properties of a family of lead-free magnetic double perovskites Cs<sub>2</sub>AgTX<sub>6</sub> (T = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu; X=Cl, Br, I). This turns out to provide an extremely fertile series, giving rise to potential candidate materials for numerous applications, viz. photovoltaic (PV), photocatalysis, spintronics etc. In conjunction with high absorption coefficient and high simulated power conversion efficiency for PV applications, few compounds in this series exhibit novel magnetic character. The distinct ferromagnetic and anti-ferromagnetic ordering driven by hybridization and super-exchange mechanism helps to break the time-reversal and/or inversion symmetry. Such a coalescence of magnetism and efficient optoelectronic response has the potential to trigger anomalous bulk/spin magnetic photovoltaic (Non-linear Optical (NLO)) effect[2] in this family, as observed recently in few non-centrosymmetric materials as well, exhibiting photovoltage larger than the bandgap. These insights can thus channelize the advancement of perovskites in magnetic-spin and/or ferroelectric anomalous PV field.

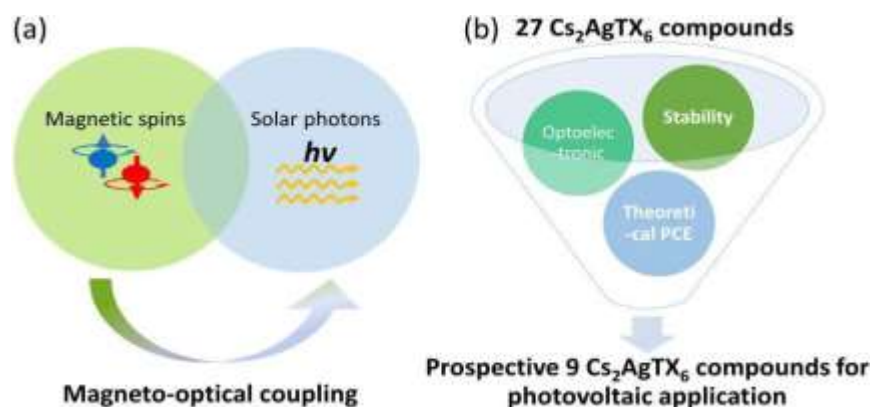


Figure 1 Schematic illustration: (a) context of the research idea (b) methodology and outcome

[1]B. Endres, M. Ciorga, M. Schmid, M. Utz, D. Bougeard, D. Weiss, G. Bayreuther & C.H Back, *Nat. Commun.* (2013), 4, 2068.

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# Innovative concepts to improve optical gain in CsPbBr<sub>3</sub> perovskite thin films

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Perovskite semiconductor thin films are major contenders for non-epitaxial laser diodes in next generation displays and optical communication devices. Understanding the gain mechanism of perovskite semiconductors is important for improving the optical gain and lasing performance. Herein, we will present different strategies to enhance optical gain of CsPbBr<sub>3</sub> perovskite thin film via controlling the excited state species, applying an external electric field, and managing the charge carrier density via an energy cascade 2D/3D perovskite heterostructure.

First, we report on routes to enhance the density of free charge carriers by increasing the average quantum well width in quasi-2D CsPbBr<sub>3</sub> thin films. The best optical gain of our quasi-2D CsPbBr<sub>3</sub> thin films is achieved by minimizing the density of photogenerated excitons, which cause serious Auger recombination losses [1].

Second, we demonstrate that the optical gain of free charge carriers in 3D CsPbBr<sub>3</sub> perovskite can be further improved by applying an external electric field. The mobile ions are directed out of the photocarrier recombination zone, which mitigates the ionic defects related non radiative recombination losses and increases the free carrier radiative recombination [2]. Moreover, we fabricate a type I perovskite-perovskite planar heterojunction with energy cascade structure using lamination technique. The low band gap 3D CsPbBr<sub>3</sub> perovskite thin film serves as the carrier sink via carrier transfer inside the heterojunction. Improved carrier and optical confinement in the newly designed planar heterojunction enhance the optical gain and reduce lasing thresholds [3]. Our strategies advance the development of low threshold perovskite semiconductor lasers both under optical excitation and electrical injection.

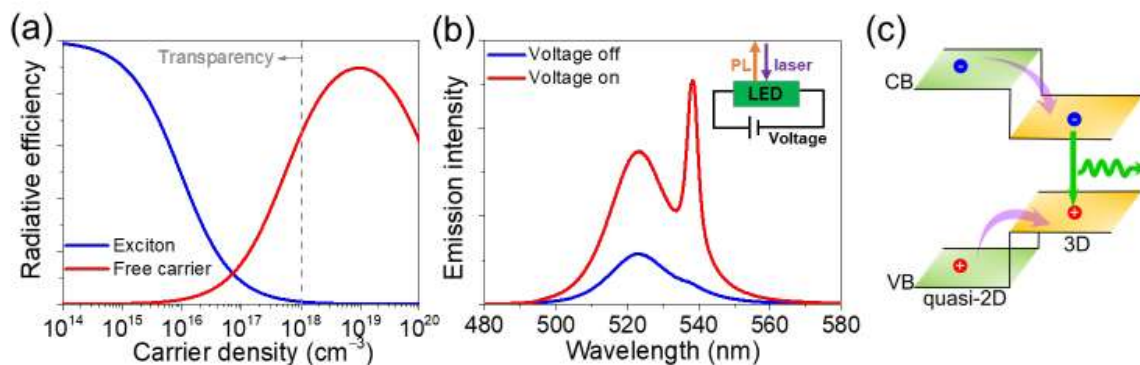


Figure 1 Innovative concepts to improve optical gain in CsPbBr<sub>3</sub> perovskite via (a) controlling excited state species, (b) external electric field and (c) planar heterojunction.

[1]Y. Li, et al., *Materials Today* (2021), 49, 35–47.

[2]Y. Li, et al., *Adv. Funct. Mater.* (2022), 32, 2200772.

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# Bandgap Engineering of Two-Step Processed Perovskite Top Cells for Application in Perovskite-Based Tandem Photovoltaics

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Tandem solar cells can raise the efficiency above the practical efficiency limit of single-junction silicon photovoltaics (PV) [1]. Wide-bandgap perovskite top solar cells (PSCs) are the perfect partners for silicon bottom solar cells given favorable optoelectronic properties and a tunable bandgap [2]. In order to maximize performance, perovskite/silicon tandem solar cells with textured front-side silicon cells are considered a highly promising architecture with the highest estimated energy yield [3]. However, to avoid shunting through the perovskite top solar cell and simultaneously ensure high power conversion efficiency (PCE), the perovskite thin films need to be processed reliably and without any pin holes over  $\mu\text{m}$ -sized pyramidal textures. Conformal coverage and growth of the perovskite layer as well as a sufficient layer thickness are indispensable [4]. The two-step method, comprising the subsequent deposition of the Pb-containing precursor materials and the organic cations, enables high film quality and the possibility of upscaling [5]. However, to date bandgap engineering for wider bandgaps ( $E_g > 1.65\text{eV}$ ) in the two-step sequential deposition is still underexplored [6]. In this work, we investigate different strategies of increasing the bandgap of perovskite top solar cells processed via two-step sequential deposition. We show that the route for adding bromide in the precursor system, i.e. in the organic cation solution and/or the inorganic  $\text{PbI}_2$  solution, is critical for the optoelectronic quality and the bromide incorporation into the perovskite thin film. By adding bromide in both of the deposition steps, the device performance - PCE of 17.2%, fill factor (FF) of 76%, open-circuit voltage ( $V_{\text{OC}}$ ) of 1.206 V and short-circuit current density ( $J_{\text{SC}}$ ) of  $18.72\text{ mA/cm}^2$  - and film quality can be maintained for  $E_g \approx 1.68\text{ eV}$  compared to the low bandgap case. Furthermore, the  $V_{\text{OC}}$  and  $J_{\text{SC}}$  of the champion devices are superior in comparison to our other studied approaches for incorporating bromide into only one of the solutions. In summary, we prove that the addition of bromide into both solutions (the organic cation solution and the inorganic  $\text{PbI}_2$  solution) leads to superior performance of PSCs. Additionally, we show that additives can improve the PCE and our optimized perovskite composition can be successfully implemented on planar and textured silicon bottom solar cells for 2T tandems.

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# Characterization of perovskite layers using photoconductance techniques

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As the perovskite materials are about to dominate the solar market both as single absorber and as tandem cells, their in-line and off-line characterization is attracting increasing interest. In this work we present how characterization techniques, already proven in other industry segments, can be applied for quality testing of the perovskite layers.

Photoluminescence (PL) techniques are applied for different purposes. While the inline imaging PL has been proven to be very useful for the rapid homogeneity testing of the deposition processes at the speed of typical production lines, recording the transient decay of the PL emission after a sub-nanosecond rapid excitation provides more detailed analysis of the carrier recombination dynamics.

Besides to transient PL, photoconductance decay measurements has been performed as well, using a microwave antenna. The longest decay component from both methods lies in the 200-300 ns range. It indicates that the decay characteristics are governed by ordinary recombination events and not the emission from trap states, and therefore applicable to test the electronic performance of the perovskite layers.

Hall measurement is a well-known technique to characterize the electrical properties of the solar materials, like sheet resistance, concentration and mobility of the majority carriers. AC magnetic field measurement based on rotating parallel dipole line system enables the measurement of the low mobility perovskites. The carrier-resolved photo-Hall addition can reveal the properties of the minority carriers as well, including the mobility, lifetime and diffusion length [1]. This enables the possibility to compare the Hall measurement with the other photoconductance methods.

Since the results measured by the imaging PL and the transient methods agrees very well, we can present a complete electrical characterization of the perovskite layers including off-line destructive measurement and in-line mapping.

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# Characteristics of Stable Inorganic CsPbI<sub>3</sub> Perovskite films deposited by thermal evaporation

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Inorganic perovskites based on CsPbI<sub>3</sub> have been studied to address the high-temperature stability and moisture stability issues of organic perovskite such as MAPbI<sub>3</sub> [1]. However, CsPbI<sub>3</sub> exhibits instability in the  $\alpha$ -phase, resulting in a phase transition to the  $\delta$ -phase (yellow phase). Recent studies have reported that the  $\beta$ - and  $\gamma$ -phases exhibit similar characteristics to the  $\alpha$ -phase [2]. Moreover, vacuum deposition has emerged as a promising method to address the limitations of spin coating, reproducibility and large-area deposition. In this study, CsPbI<sub>3</sub> was deposited by the co-evaporation or sequential-evaporation of CsI and PbI<sub>2</sub>. The molar ratio of CsI and PbI<sub>2</sub> was controlled the deposition rate through QCM monitoring system to investigate the characteristic changes under Cs- rich and Pb-rich conditions. Furthermore, by controlling the substrate temperature (<150°C), we observed the phase transition during the as-deposited phase and the phase transformation induced by post-deposition annealing (PDA). The deposited CsPbI<sub>3</sub> exhibited a bandgap of 1.75 eV and the presence of the  $\gamma$ -phase, as confirmed by PL, UV- vis, and XRD analyses. The stability of the CsPbI<sub>3</sub> in black phase ( $\alpha$ ,  $\beta$ , or  $\gamma$ -phase) was improved by optimizing the substrate and PDA temperature.

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[2] Julian A. Steele et al., *Science* (2019), 365, 679-684.

# Pulsed laser deposition of inorganic halide perovskite thin films with various compositions

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Micro-LEDs are often described as the most promising technology to improve large displays quality and to realize high-brightness micro-displays for augmented and mixed reality. However, fabrication of full colour micro-LEDs pixels, with a pitch under 5 $\mu$ m, is challenging and various solutions are considered. Among them, the deposition of colour conversion layers above blue micro-LEDs to produce red and green emission is studied [1]. Achieving high luminance (10<sup>6</sup>cd/m<sup>2</sup>) and high colour purity is desirable for micro-LEDs displays [2]. Inorganic halide perovskite materials are interesting candidates as colour conversion layers. Indeed, they are semiconductors with a direct bandgap, a high absorption coefficient and a narrow spectral emission. Moreover, they offer the possibility to tune their bandgap by changing the composition, thus covering the entire visible spectrum.

Diverse deposition processes can be used to deposit inorganic perovskite thin films. Among them, pulsed laser deposition (PLD) is an interesting option. Indeed, PLD is compatible with deposition over large surface such as wafer 200 and 300mm. Furthermore, during deposition, the stoichiometry of the target is largely transferred to the thin film, thus enabling a fine control of the perovskite composition [3].

Here we report the deposition of perovskite thin films by PLD with various compositions: CsPbBr<sub>3</sub>, CsPbI<sub>2</sub>Br and CsPbI<sub>3</sub>. Different parameters have been tested for deposition of layers on top of 200mm SiO<sub>2</sub> wafers, leading to the obtention of a pure red and green emission. Morphological, crystallographic and optical characteristics have been studied. Finally, photoluminescence properties have been measured over time to record perovskite stability under different conditions (air exposure, encapsulation layer protection...).

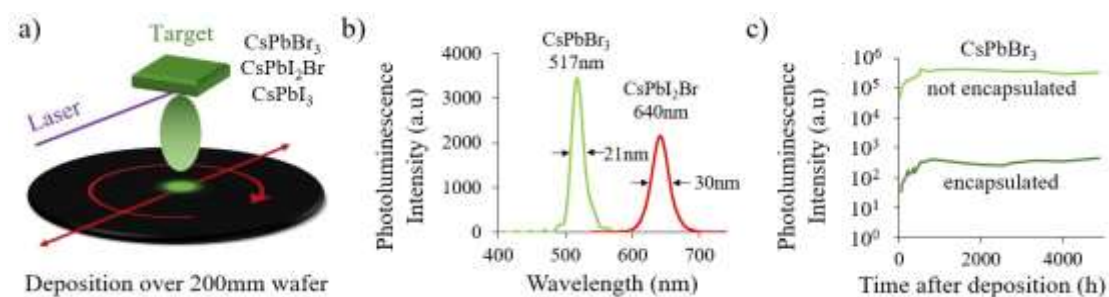


Figure 1 – a) PLD deposition process, b) Photoluminescence of perovskite thin films, c) Evolution of the photoluminescence intensity along time for CsPbBr<sub>3</sub> thin films.

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# Analog Memristor of Cs<sub>4</sub>CuSb<sub>2</sub>Cl<sub>12</sub> Perovskite Nanocrystals as Solid- State Electronic Synapse

Sumaiya Parveen<sup>1</sup>

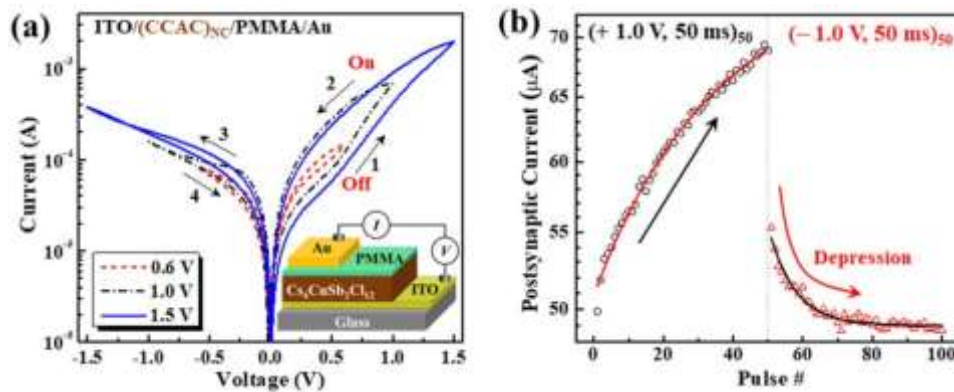
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Brain-inspired artificial neural networks and neuromorphic computing are taking space to a new height based on solid-state memristor devices. Despite considerable progress already made, the use of lead-free double perovskite materials with direct bandgap can be recognized as a significant paradigm shift in this field. In this study, we have conducted a comprehensive investigation into the growth, thin film deposition, and analog electroforming-free resistive switching properties of lead-free layered caesium copper antimony chloride (Cs<sub>4</sub>CuSb<sub>2</sub>Cl<sub>12</sub> or CCAC) double perovskite nanocrystals (NCs)[1]. Optical and structural characterizations of CCAC NCs confirm the growth, the existence of direct bandgap, and <111> oriented monoclinic crystal phase of space group C2/m. Systematic current–voltage (*I–V*) characteristics confirm the robust electroforming-free resistive switching property with high endurance over 2×10<sup>3</sup> cycles and it displays enhanced memory window by increasing ±*V*<sub>Max</sub> values, say 0.6, 1.0, and

1.5 V (Figure 1(a)). Figure 1(b) illustrates the potentiation and depression of synaptic connection strength, as indicated by recorded postsynaptic currents, encompassing both excitatory and inhibitory responses. This modulation is achieved through programming the presynaptic terminal with 50 consecutive positive or negative pulses, replicating synapse-like states. Hence, the single memristor device composed of CCAC NCs showcased in this study exhibits the ability to perform simultaneous data processing and storage, while also emulating a range of synaptic and neural functions.



**Figure 1.** (a) Current–voltage (*I–V*) characteristics of perovskite resistive switching devices in loops by sweeping voltage starting from zero to +*V*<sub>Max</sub> to -*V*<sub>Max</sub> to zero again. (b) Potentiation and depression of synaptic connectivity or weight recorded by applying consecutive 50 write (+1.0 V, 50 ms) pulses first and then 50 erase (-1.0 V, 50 ms) pulses, respectively. Lines represent theoretical fitting using exponential grow (red line) and decay (black line) functions.

# Boosting device performance of low-dimensional perovskite solar cells by ionic liquid engineering

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In the vast research domain of perovskite solar cells (PSCs), efficiency and stability are often on the two extremes for better-performing devices [1]. The three-dimensional PSCs are capable of having better efficiency, but they compromise in terms of stability, whereas the low-dimensional perovskites that ace stability have comparably low efficiency [2,3]. In this work, we studied the impact of ionic liquid as an interlayer for better efficiency and stability of low-dimensional PSCs. The Phenethylammonium-based low-dimensional Ruddlesden-Popper (RP) perovskite ((PEA)<sub>2</sub>MA<sub>4</sub>Pb<sub>5</sub>I<sub>16</sub>) shows an efficiency of 9.73% with the pristine device. However, the addition of ionic liquid as an interlayer improves the efficiency to 11.56% by majorly enhancing the short-circuit current. The ionic liquid not only gives a remarkable increment in efficiency but also improves stability to a significant extent. The unencapsulated films, with and without ionic liquid modification, are kept in an ambient atmosphere at 80 °C with a relative humidity of 35% and are studied for degradation. The bare films underwent complete degradation in 300 mins, whereas the treated films showed only slight degradation in the same time frame. It is interesting to note how ionic liquid enhances both stability and efficiency by catering to the relevant factors, hence enabling us to get the best of both.

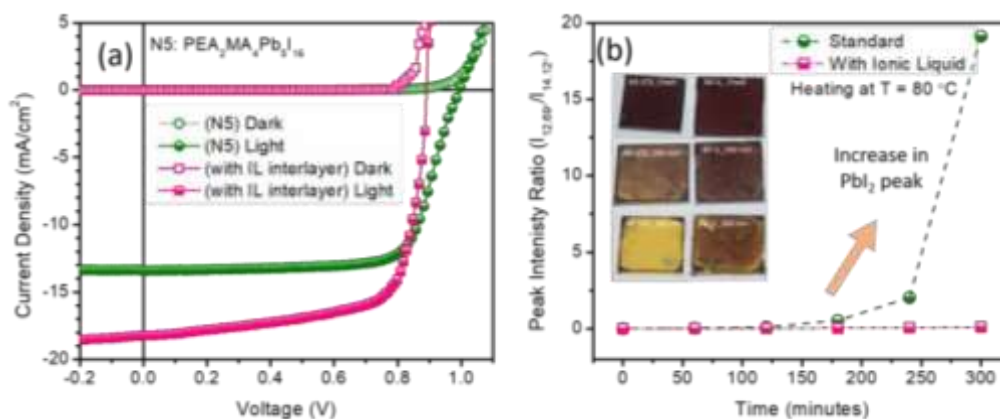


Figure 1 (a). J-V characteristics of (PEA)<sub>2</sub>MA<sub>4</sub>Pb<sub>5</sub>I<sub>16</sub> (N5) standard and ionic liquid modified PSCs, (b). Thermal stability of unencapsulated (PEA)<sub>2</sub>MA<sub>4</sub>Pb<sub>5</sub>I<sub>16</sub> standard and ionic liquid modified perovskite thin films at 80 °C in ambient conditions.

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# Synthesis of CsPbBr<sub>3</sub> Nanocrystals Employing a New X-Type Ligand Based on Sulphur-atom.

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Lead halide perovskite nanocrystals have drawn attention in the recent years due to its optoelectronic properties that makes it suitable for various applications such as photodetectors, light emitting diodes and photovoltaics.<sup>[1][2]</sup> Here, we have developed a new X-type surface ligand (**MP-LS1**), based on sulphur -atom for synthesis of CsPbBr<sub>3</sub> nanocrystals.<sup>[3]</sup> The synthesis of the ligand was performed via the nucleophilic substitution reaction to obtain the pure ligand, which was subsequently engaged for CsPbBr<sub>3</sub> nanocrystal synthesis using ligand assisted reprecipitation technique at room temperature and hot-injection method.<sup>[2]</sup> The tuning of the perovskite nanocrystal size was also acquired through different synthesis method.<sup>[4]</sup> This resulted in the perovskite nanocrystals with > 90% photoluminescence quantum yield (PLQY) and decent stability at ambient conditions.

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# Mitigating performance losses in perovskite solar cells incorporating ionic transport layers

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Poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) is a frequently applied hole transport layer (HTL) in organic solar cells. Its use in perovskite solar cells (PSCs), however, has been primarily limited to lead-tin and tin-only devices due to the significant open circuit voltage ( $V_{OC}$ ) losses it has shown in Pb-only devices. [1,2] These losses are typically attributed to the energy level mismatch between PEDOT:PSS and the perovskite, however, such losses are not observed in PSCs employing other hole selective contact modifiers and in organic photovoltaic devices where similar energy level mismatch exists.

In this work, we provide an understanding of the loss mechanisms in PEDOT:PSS based devices and examine methodologies to mitigate them during the device processing stage. We have chosen methylammonium lead iodide ( $MAPbI_3$ ) for this study, as it eliminates the possibility of interference from other factors such as phase segregation effects, oxidation of tin, etc. which are present in more complex perovskite compositions. [3-5] The controlled crystallization of the perovskite is identified to be an important factor which strongly affects the performance of  $MAPbI_3$  devices incorporating PEDOT:PSS as its HTL. We show the potential for significant improvements in the PCE (as high as ~50%) through careful recrystallisation of the perovskite absorber. These performance enhancements are further discussed in the context of structural improvements realized and its impact on the optical and electronic properties of the perovskite absorber.

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# Nanoparticles for improved wettability and enhanced carrier lifetimes of perovskites on hydrophobic self-assembled monolayers

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The incorporation of hole selective self-assembled monolayers (SAMs) has proven to be a promising approach towards realizing both high efficiencies as well as improved stability in inverted perovskite solar cells (PSCs). [1,2] Out of the several SAMs developed, the carbazole based methyl substituted SAM, [4-(3,6-Dimethyl-9H-carbazol-9-yl)butyl]phosphonic Acid (Me-4PACz), has been employed in many of the record efficiency devices achieving power conversion efficiencies (PCEs) exceeding 32% for perovskite/Si tandem devices. [2,3] However, the poor wettability of the perovskite on the non-polar Me-4PACz surface has been reported by several groups and has proven to be the main bottleneck in the widespread deployment of this SAM in PSCs. [4,5] In this work, we demonstrate the use of alumina (Al<sub>2</sub>O<sub>3</sub>) nanoparticles (NPs) as pinning sites for perovskites on Me-4PACz, which allows the realization of a complete, pin hole-free coverage of the perovskite and thereby, an improved device yield. [6] Further, this Al<sub>2</sub>O<sub>3</sub> NP based modification of Me-4PACz is shown to result in significantly enhanced Shockley-Read-Hall recombination lifetimes exceeding 3 μs in perovskites formed on it, as compared to those formed on unmodified Me-4PACz and those modified with a commonly adopted interfacial compatibilizer, poly[(9,9-bis(3'-((N,N-dimethyl)-N-ethylammonium)-propyl)-2,7-fluorene)-alt-2,7-(9,9-dioctylfluorene)]dibromide (PFN-Br). Devices fabricated on Al<sub>2</sub>O<sub>3</sub> NP based modification of Me-4PACz are demonstrated with PCEs of ~20%, which is a >20% improvement in PCE to those fabricated on Me-4PACz modified with PFN-Br. Finally, we show that, while PFN-Br modified devices reach their T<sub>80</sub> at 160 h after being stored under open circuit conditions in the dark at 65 °C in ambient environment, Al<sub>2</sub>O<sub>3</sub> NP modified devices retain more than 90% of their initial PCE for the same duration.

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# Asymmetric triphenylethylene-based hole transporting materials for highly efficient perovskite solar cells

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Perovskite solar cells (PSCs) have undoubtedly become the super star in the photovoltaic field, and now the certified power conversion efficiency (PCE) has reached a very high level of 26.0%, which is comparable to that of the most commercially common crystalline silicon solar cells [1].

An important component of the PSC is the hole transporting material (HTM) which determining the cost, energy conversion efficiency and longevity of the device [2]. However, most HTMs suffer from drawbacks such as complex and costly synthesis, self-aggregation that degrades hole transport layer quality, and decreases device stability and efficiency. Hence, efforts continue to develop improved HTMs with advantages such as compatibility with perovskite valence and conduction bands, minimal absorption in solar spectrum, sufficient hole mobility, thermal and photochemical stability, processability, and low cost.

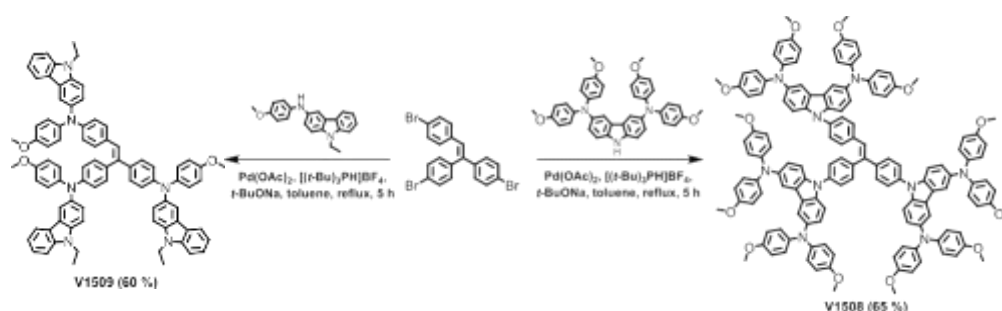


Figure 1. Synthesis of HTMs V1508 and V1509.

In this work we describe the synthesis and application of new HTMs (**V1508** and **V1509**) comprised of triphenylethylene central core and carbazole derivatives as substituents. These materials can be obtained in facile two or three-step synthesis procedure. Their thermal, optical, and photoelectrical properties are thoroughly documented. The new materials were tested as HTMs and successfully applied in PSCs, reaching efficiencies above 23%. Furthermore, the device employing the best performing HTM **V1509** compound demonstrated improved long-term stability compared to PSCs with spiro-MeOTAD as a HTL.

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# How Substrate Surface Passivation Dictates Preferential Growth of Thermally Co-Evaporated Perovskite Thin Films

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Hybrid metal halide perovskite solar cells have achieved remarkable efficiency levels, approaching market-dominating silicon solar cells.[1] Low fabrication costs and potential integration into tandem solar cells make them an appealing choice for highly efficient next generation photovoltaics. Commercialization requires a uniform, scalable and reproducible deposition. Thermal co-evaporation under high vacuum of perovskite precursor materials is a particularly promising process, allowing high control of perovskite composition and thickness on large areas. Recently, our group developed a process for vacuum deposition of nearly lossless carbazole-based (nPACz) self-assembled monolayer hole transport layers (SAM-HTLs).[2,3] We adapted the methodology to fabricate fully evaporated perovskite solar cells. Here we found stark differences of perovskite crystallization behavior depending on the fabrication method of the SAM-HTL layer. In our previous work we found that crystallization of MAPI films is highly dependent on the choice of substrate material.[4] However, a deeper understanding of the involved mechanisms is still lacking. In this work, we study and compare perovskite film growth of co-evaporated perovskite material with a composition of Cs<sub>0.15</sub>FA<sub>0.85</sub>Pb(I<sub>2.7</sub>Cl<sub>0.3</sub>) on solution processed and evaporated SAM-HTLs. We find that the perovskite growth is strongly affected by the thickness of nPACz derivatives and observe a selective formation of the desired photoactive perovskite alpha phase for thicker layers. In depth investigation of this stabilization mechanism was performed by a combination of synchrotron X-ray emission (XES)- and nuclear magnetic resonance (NMR) spectroscopy and further supported by theoretical investigation based on density functional theory. We believe that the unraveled mechanism is of fundamental nature and transferable to different HTL/perovskite interface systems. Based on our results, we will further explore different approaches to rationally tune the surface chemistry, enabling precise control of perovskite growth.

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# Advanced Laser-Patterned Interconnection Concepts for Perovskite (Tandem) Solar Modules

Julian Petry

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Considering global warming and the global energy crisis, exploiting the full potential of photovoltaics (PV) through research and innovation is crucial for the rapid transition to a renewable and resilient energy supply system. Next generation perovskite-based thin-film PV opens up new opportunities. The technology is driven by outstanding optoelectronic properties, bandgap tunability and solution-based processability of perovskite semiconductor thin films. In this contribution, we present our latest advances on laser patterned perovskite solar modules. We will report on three aspects: (i) laser patterned scalable two-terminal all-perovskite tandem solar modules, (ii) laser patterned translucent perovskite solar modules for building integration, and (iii) the application of back-end interconnections in perovskite solar modules. All-perovskite tandem solar modules: Perovskite tandem PV promises to surpass the Shockley-Queisser efficiency limit of single-junction solar cells while also providing the advantages of cost-efficient all-thin-film technologies. Recent advances in lab-scale two-terminal all-perovskite solar cells make the transfer to scalable manufacturing methods for fabrication of solar modules the next essential step for commercialization. Here, we show the first all-perovskite tandem module exclusively with scalable fabrication methods (blade-coating, vacuum deposition), resulting in solar modules of 12.25 cm<sup>2</sup> aperture area that demonstrate power conversion efficiencies (PCEs) above 19% [1]. The interconnections were realized via cost-efficient nanosecond pulsed laser system in inert atmosphere, enabling residue-free ablation and high geometrical fill factors of >94%. Translucent perovskite solar modules: Besides opaque modules, we present micropatterned translucent all-perovskite tandem solar modules for building integration fabricated via a scalable laser scribing process [2]. In-depth optical analysis and viewthrough images prove neutral color rendering, minimal haze, and homogeneous optical impression. Record two-terminal perovskite-perovskite tandem solar cells exhibit >11% PCE for >30% average visible transmittance. Furthermore, the novel concept of arbitrary transmittance gradients is presented, enabling new architectural possibilities for building-integrated photovoltaics.

Back-end laser patterned solar modules: Lastly, the modern demand for individualization is addressed by application of back-end interconnections. Realizing interconnections after deposition of functional layers, any individualization can be deferred to a downstream machining step and does not affect the complexity of the standard process. Here, we present the feasibility of back-end interconnections for perovskite solar modules and demonstrate advanced interconnections schemes based on scalable fabrication processes, enabling GFF improvements and reduced parasitic losses.

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# Effect of charge extraction layer on optoelectronic properties of perovskite via Photoluminescence Imaging

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Over the last few years, powerful numerical simulations have been developed that give clear guidelines on how to analyze and interpret photoluminescence transients measured on perovskite absorbers, including extraction layers [1]. We used absolute photon-calibrated hyperspectral photoluminescence imaging and time-resolved photoluminescence (TRPL) imaging to better understand the lateral inhomogeneities in state-of-the-art perovskite absorbers as well as provide insights into the interfacial charge transfer and recombination processes. In this work, we study  $(\text{FAPbI}_3)_{0.97}(\text{MAPbBr}_3)_{0.03}$  deposited on mesoporous  $\text{TiO}_2$  with and without an organic passivation layer. The samples reached power conversion efficiencies of 24% for the passivated and 22.7% for the unpassivated case. We measured TRPL on the two interfaces: perovskite/air and m- $\text{TiO}_2$ /perovskite of unpassivated and passivated surfaces to distinguish between surface recombination, interface recombination, and charge extraction. The TRPL transients measured from the perovskite side are different from the ones measured from the glass side (Figure 1). The initial fast decay we see in the case of glass side illumination is attributed to the effect of electron transfer to the ETL layer which changes the  $np$  product in perovskite bulk thus reducing PL. We find that the effect of the charge extraction is spatially modulated due to an inhomogeneous  $\text{TiO}_2$  deposition.

Our results show that the m- $\text{TiO}_2$  layer is not ideal for the highest-performing solar cells since the electronic properties are spatially modified with leads to changes in quasi-Fermi-level splitting, minority carrier lifetime, and consequently also in open-circuit voltage.

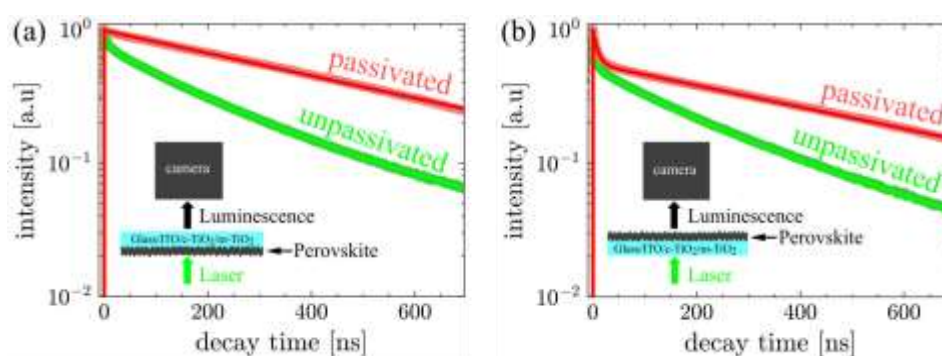


Figure 1: Photoluminescence at 532nm pulsed laser of the perovskite, (a) illuminated from the perovskite/air interface. (b) illuminated from the glass side ( $\text{TiO}_2$ /perovskite interface).

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# Interface study between transport layers by atomic layer deposition and FA-based perovskites

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The incorporation of perovskite solar cells as a top cell in a tandem solar cell structure holds great potential in pushing the efficiency limits. The best performing perovskite/silicon or perovskite/CIGS tandem solar cells utilize a p-i-n perovskite solar cell configuration with a combination of evaporated C<sub>60</sub> and atomic layer deposition (ALD) based tin oxide (SnO<sub>x</sub>) as electron transport layers (ETL) [1,2]. Owing to the superior qualities of ALD-based inorganic films, such as their robust, pin-hole free, uniform, and conformal nature, they can improve the performance, and stability by protecting the layers underneath, of a perovskite solar cell structure. These layers also act as buffer layers and prevent damage to the perovskite layer from the successive sputtering of transparent conductive oxide (TCO). Due to the high reactivity of ALD precursors, direct deposition of transport layers on top of perovskites can have adverse effects on the surface of the perovskite layer. One such example was demonstrated by A. Hultqvist *et al.*, where direct deposition of ALD-based SnO<sub>x</sub> on top of Cs<sub>0.05</sub>FA<sub>0.79</sub>MA<sub>0.16</sub>PbBr<sub>0.51</sub>I<sub>2.49</sub> (perovskite) lead to the formation of a non-ideal interface containing new chemical environments [3]. Often, C<sub>60</sub> is employed as an interlayer between perovskite and ALD SnO<sub>x</sub> to prevent the formation of an undesired interface and allow unobstructed transport of charge carriers.

However, the use of organic transport layers such as C<sub>60</sub> can also have several downsides from a cost and stability point-of-view. Therefore, solely using inorganic transport layers would be preferable, if they could form high quality interfaces to the perovskite. This study investigates this possibility by looking at the interface between pristine FA-based perovskite absorbers and ALD-based SnO<sub>x</sub> as ETL. Mainly the influence of halides (I and Br) in the formation of the interface at FAPbBr<sub>3</sub>/SnO<sub>x</sub> and FAPbI<sub>3</sub>/SnO<sub>x</sub> is investigated by employing hard x-ray photoelectron spectroscopy (HAXPES) technique. Learning the reactivity of the precursors used in an ALD process, in this case tetrakis(dimethylamino)tin (TDMASn) and H<sub>2</sub>O, towards different perovskite compositions will pave the way toward achieving high-quality interfaces by direct deposition of inorganic transport layers such as ALD SnO<sub>x</sub> on perovskites.

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# Pronounced Room-Temperature Vibrational Coherence Coupled to Electronic Transitions in Cs<sub>2</sub>Au<sub>2</sub>Br<sub>6</sub>

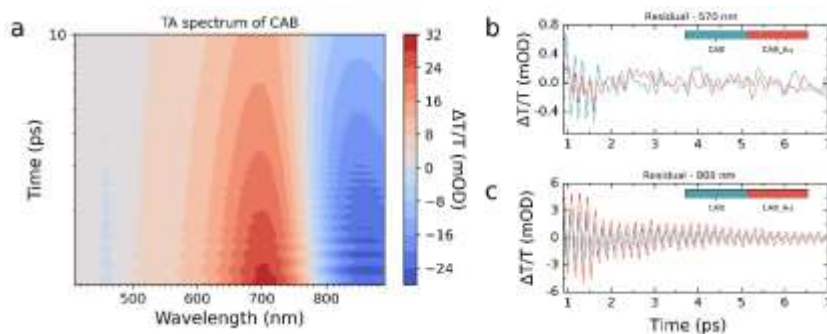
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Cs<sub>2</sub>Au<sub>2</sub>Br<sub>6</sub>, a double-perovskite semiconductor is studied as an alternative to conventional lead-based halide perovskites that are known for their toxicity and limited stability. The optical properties of Cs<sub>2</sub>Au<sub>2</sub>Br<sub>6</sub> are investigated using steady-state and time-resolved spectroscopies. The absorption spectra are characterized by inter-valence charge transfer transitions due to the mixed valency of Au ions in the double perovskite[1]. Pump-probe measurements at room-temperature reveal oscillations in the spectrum lasting several picoseconds. This points to vibrational coherences via optical phonons coupled to the electronic transitions as the origin of the oscillations, which is further elucidated. When doped with Au nanoparticles, the Cs<sub>2</sub>Au<sub>2</sub>Br<sub>6</sub> films show a modulation of their electronic properties while still exhibiting the oscillations. However, the oscillations are suppressed at the plasmonic resonance frequency of Au nanoparticles, indicating an interplay of plasmons and phonon modes in the perovskite. The rich electronic and vibrational properties of Cs<sub>2</sub>Au<sub>2</sub>Br<sub>6</sub> and their modulation by Au nanoparticles highlight their potential for optical and photonic technologies.



**Figure 1: (a) Transient absorption spectrum of Cs<sub>2</sub>Au<sub>2</sub>Br<sub>6</sub> (CAB). (b- c) Residual oscillatory dynamics extracted from the TA spectra compared for undoped and Au-doped Cs<sub>2</sub>Au<sub>2</sub>Br<sub>6</sub> (CAB\_Au) at different probe wavelengths: 570 nm (b) and 800 nm (c).**

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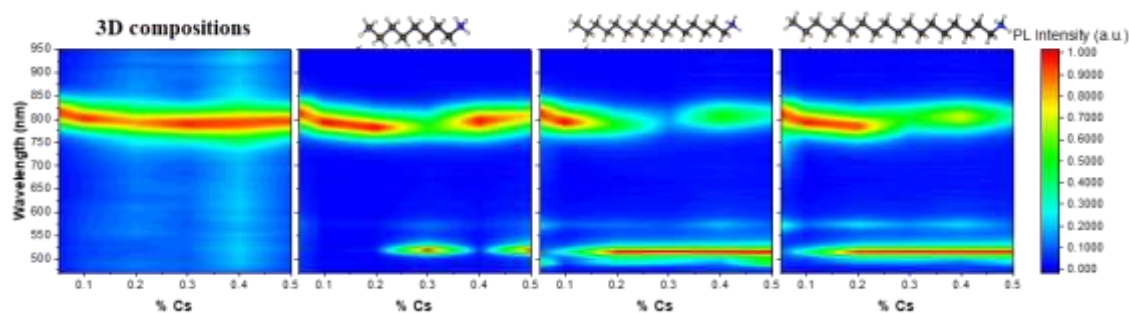


# The influence of the chemical composition of 3D perovskites on the formation and stability of 2D/3D structures

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The formation and stability of 2D/3D perovskite structures are crucial for understanding their properties and optimizing their performance. The primary distinction between 2D and 3D perovskites lies in the dimensionality of their crystal structures. 3D perovskites are formed by an extensive three-dimensional network of corner-sharing octahedra, while 2D perovskites consist of multiple layers of organic cations sandwiched between inorganic lead halide layers. [1] The synthesis of 2D/3D perovskites involves intricate chemical techniques. In the case of 2D perovskites, the choice of organic cations and their structure significantly impacts the formation and stability of the material. [2] The size and shape of the organic cations determine the layer thickness, and their interactions with the inorganic layers influence the overall structure's stability. Precise control over synthesis parameters is essential to achieve well-crystallized and uniform 2D structures. Understanding the stability of 2D/3D perovskites is critical for their application in solar cells and other optoelectronic devices. Researchers aim to enhance efficiency, durability, and reliability by manipulating the composition and structure of perovskite materials. Additionally, the combination of 2D and 3D perovskite structures exhibits unique properties, such as improved stability and adjustable bandgaps, paving the way for advanced device architectures and customized optoelectronic applications. [3] In this study, the influence of composition and chain size on 2D formation and stability was investigated. Figure 1 displays a photoluminescence (PL) mapping of films prepared with varying compositions of 3D perovskites and different cations for 2D formation. The relationship between cesium and formamidinium affects the formation of the 2D structure and the specific types that can be formed. Additionally, the chain size exhibits a distinct influence on the formation process.



**Figure 1. The mapping of 3D perovskites pure, and with different compositions, using octylammonium, hecacylammonium, and octadecylammonium, for the formation of 2D/3D structures.**

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# Monolithic Perovskite/Silicon Tandem Solar Cells Prepared by Thermal Co-Evaporation with Optimized Top Cell Band Gap

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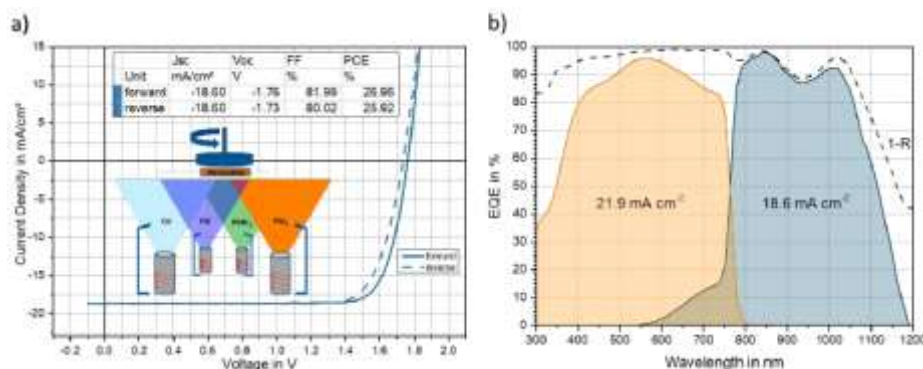
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Monolithic perovskite/silicon tandem solar cells (PSTSCs) have recently achieved power conversion efficiencies above 32% using spin coated metal halide perovskite.[1] However, solution-based deposition of perovskites involves a number of limitations. In particular, conformal coverage of textured surfaces or composition gradients in the absorber material can hardly be realized. These limitations can be overcome with vacuum-based deposition techniques such as thermal co-evaporation. So far, mainly co-evaporated perovskite solar cells with iodine rich compositions were reported,[2] resulting in absorbers with band gaps below 1.63 eV, which is not ideal for PSTSCs.

In this work, we focus on the vacuum-based preparation of perovskites solar cells with band gaps between 1.63–1.70 eV using mixtures of formamidinium iodide, lead iodide, lead bromide, and cesium iodide co-evaporated from four individual sources. We analyze how film stoichiometry, substrate temperature, and annealing conditions influence the morphology and photoluminescence quantum yield of the formed perovskite absorbers. By using an optimized annealing procedure and a perovskite composition with a cesium content below 25% relative to lead, phase stable front side planar monolithic PSTSCs with a PCE of over 26.5% were achieved. To reduce the reflection losses for wavelengths above 700 nm shown in Figure 2b the co-evaporation process can be used to conformally cover bottom cells with random pyramid textures. Our results demonstrate that the herein reported co-evaporation process is suitable to form phase stable wide band gap perovskites absorbers, enabling efficient and industrial relevant PSTSCs with scalable processing.



**Figure 1: a) Current density–voltage characteristics of a perovskite (~1.65 eV) /silicon tandem solar cell with a schematic of the co-evaporation process in the inset. b) Corresponding external quantum efficiency spectra together with 1-reflection.**

# Wind effects on the performance and hysteresis of building-integrated perovskite solar cells

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Perovskite solar cells (PSCs) are thin-film semitransparent, flexible, and color-tunable photovoltaic technologies with high optoelectronic efficiency. Therefore, they can be used in different sites of buildings, such as envelopes, walls, window facades, rooftops, etc. In this perspective, integrating PSCs with either conventional or unconventional sites of buildings can more quickly pave the transition pathway from fossil fuels to renewable energy sources. However, the characterization of the operating performance of PSCs for building applications is typically hindered by their long-term stability, the meteorological data, and the complex nature of the wind flow. This study investigates the wind effects on the performance and hysteresis of building-integrated perovskite solar cells (BIPSCs) under different meteorological conditions.

The performance and hysteresis characteristics of BIPSCs significantly differ from those outlined for a PSC under the standard testing condition (i.e.,  $T_{amb}=25^{\circ}\text{C}$  and 1-Sun illumination). The difference mainly originates from the three following key factors: (i) meteorological data, (ii) spatial and temporal distribution of wind due to the turbulent nature of the wind intensity and the wind flow pattern in urban areas, and (iii) the integration of cells to form a module for installation, which can impact the resultant electrical output delivered to the grid networks.

The present study uses a multi-physics computational model to investigate the effects of wind flow on the optical, electrical, and thermal performance of PSCs, integrated into a building, under different meteorological conditions. The study also specifies the effects of wind speed and its direction on ion migration and hysteresis of each cell. The developed multi-physics computational model consists of (i) a mathematical model for the performance and hysteresis assessment of a perovskite solar cell under real-world operating conditions and (ii) a computational fluid dynamics (CFD) framework to characterize wind flow effects around a standalone building. For the former, a coupled optical-electrical-thermal model is developed based on drift-diffusion and Poisson's equations, and later, the model is coupled with the CFD framework to include the distribution effects of exterior convective coefficient (arising from wind) in the thermal evaluation of BIPSCs. The results indicate that the cell temperature can vary more than  $15^{\circ}\text{C}$  over the surface of the building façade for FTO/TiO<sub>2</sub>/MAPI/Spiro-OMeTAD/Au cell architecture. This cell temperature difference leads to the rise of the steady-state power conversion efficiency from 19.2% to 19.9% and doubles the hysteresis rate over the building façade surface. The results of this study can provide insight into the performance and degradation characterization of perovskite solar cells for building applications that can pave the way for fast commercialization of this technology.

# Thermally Stable and Water-resistant using All-Inorganic CsPbI<sub>2</sub>Br Perovskite Solar cells

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All-inorganic perovskite solar cells (PSCs) have emerged as one of the prominent directions of the perovskite research field due to their high-temperature stability compared to their thermally less stable hybrid counterparts. One prominent example for all-inorganic perovskites are CsPbI<sub>2</sub>Br compositions. These are thermally stable and offer bandgaps, relevant for LEDs or multijunction solar cells [1]. However, they are unstable against moisture from the atmosphere, let alone direct exposure to water [2,3]. Here we show, promising stability improvements CsPbI<sub>2</sub>Br PSCs in terms of thermal, moisture, and constant light illumination using a P3HT-treated interface. Implementing the strategy, the CsPbI<sub>2</sub>Br devices retained ~50% of their initial PCE for 30 min upon direct exposure to ~60% relative humidity (RH) and ~90% of their initial PCE for 300 min with a thermal stress of 250 °C. The P3HT-based interface helped to improve the stability and device performance with the champion device going from 12.5% to 14.1% performance and a FF of 82.2%. In addition, the target devices showed outstanding water resistance upon direct exposure to water.

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# Unravelling Lead Free Perovskites for White Light Emission by Charge Carrier Localization Amongst the Lattice Structure.

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All-inorganic lead free double halide perovskites nanocrystals(NCs) have been into of prime interest amongst the researchers since last few couple of years. But their instability under the ambient conditions, low efficacy along with poor Photo- Luminescence Quantum Yield (PLQY) still remains a concern [1]. Researchers have dealt with the substitution of homovalent elements into perovskite systems in terms of doping that enhances the overall PLQY of NCs by suppressing the defect states or creating a local Self Trap Energy(STE) state [2]. Here we have proposed a divalent metal cation ( $M^{2+}$ ) substitution into the lattice sites of a monovalent and trivalent metal cation in a double perovskite namely  $A_2B'B''X_6$  NC's by using a conventional hot injection method for the very first time. Pure NCs synthesized exhibited good stability under air but unfortunately a very weak photoluminescence. In our work, this eventually is enhanced by critical  $M^{2+}$  doping that emits a cool white emission. Now in addition, NCs were combined with a red emitting lead free perovskite (B) for obtaining a stable pure white light (with CIE coordinates (0.33,0.32)). The purity and stability of the synthesized NC's were intact even after 60 days under ambient conditions which were confirmed via XRD. It is predicted that two  $M^{2+}$  atoms are replaced by each  $B'$  and  $B''$  lattice sites. Luminescence enhancement might occur due to the symmetric lattice periodicity breaking [3]. This eventually results in charge carrier localization which results in an enhanced radiative recombination and thereby PLQY of the material. Thus, a critical  $M^{2+}$  doping along with the red emitting lead free perovskite has all the necessary components with a proper weight ratio required for White Light Emission (WLE). Hence, we proposed a lead-free double perovskite system to achieve WLE, that could be a strong candidate for white LED applications and other such opto-electronic devices.

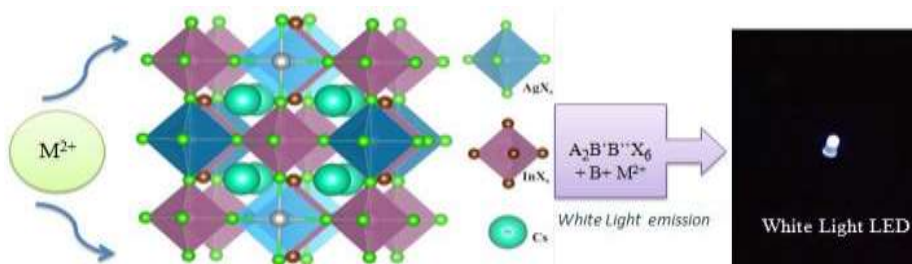


Figure 1 Schematic Diagram for White Light Emission

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# The effect of halide composition on the luminescent properties of cesium-copper halide pseudo-perovskites

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Ternary copper halide (TCH) pseudo-perovskites are potential active materials in light emission applications and extensive research is devoted to understanding their optoelectronic properties. TCHs can also be used in the efficient detection of various forms of high-energy radiation (e.g., X-rays,  $\gamma$ -rays, charged particles and fission fragments) with excellent light yield, good energy resolution, and minimal afterglow.[1] These perovskite-derived compounds also offer to remedy some of the shortcomings of their hybrid lead-halide predecessors such as: (i) ambient instability, (ii) toxicity of Pb, (iii) thermal instability, (iv) parasitic self-absorption of emitted light. The light emission process in TCH compounds involves self-trapped excitonic states (STEs) that are formed through lattice distortions after excitation. Light emission from these STE states is spectrally wide, significantly Stokes-shifted and possess long photoluminescence lifetime (generally in the microsecond time range). Similarly, to lead-halide perovskites these optoelectronic properties can be fine-tuned by the preparation of mixed-halide compositions. However, the emission from these STE states is not yet fully understood. In this presentation I will focus on the preparation of mixed-halide Cs<sub>3</sub>Cu<sub>2</sub>X<sub>5</sub> films (where X: I and/or Br) using a simple spray-coating method. With various material characterization techniques, we proved the successful preparation of mixed-halide films. We found that with increasing bromide content of the TCH films the emission process of these materials became more vulnerable to trap states, ultimately influencing the optoelectronic properties of the layers. To better understand the role of halide composition we determined the exact band structure of these compounds and translated the different processes (e.g., exciton binding and self-trapping) on the absolute energy scale by combining different spectroscopic characterization techniques (e.g., ultraviolet photoelectron spectroscopy). We also aimed to reveal whether the change in the photoluminescence properties of the layers is directly reflected in the radioluminescence response following the exposure of the TCH films to  $\alpha$ -particles from a radioactive source. The insights gained from these measurements can be used in the better design of TCH light-emitters for light and radiation detection applications.

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# Tuning the electronic structure of SnO<sub>2</sub> via Mg-doping for application in perovskite solar cells

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As of today, tin dioxide (SnO<sub>2</sub>) is considered one of the best electron transport materials for n-i-p Perovskite Solar Cells (PSCs) [1], with numerous works in the literature highlighting the beneficial role of different dopants in tuning its electronic and structural features. One example is Mg, which has been reported to increase the efficiency of SnO<sub>2</sub>-based PSCs, in particular by increasing the open circuit potential (VOC) [2] and by improving the film quality [3], when incorporated in the SnO<sub>2</sub> matrix in low concentrations. High Mg contents, instead, result in a decreased cell efficiency. In this work, we performed spin-polarized density functional theory calculations to provide new insights into the effects induced by different percentages of Mg doping. Structural, electronic and defect properties have been evaluated. Based on our results, low Mg contents push up the SnO<sub>2</sub> conduction band minimum (CBM), which justifies the increasing VOC reported in the literature. On the contrary, at high dopant concentrations, the presence of interstitial Mg defects lowers the CBM and generates structural distortions, explaining the drop in PSC performances at a high Mg doping ratio. Our analysis defines a new atomistic perspective on the reasons behind the positive/negative impact of Mg doping in SnO<sub>2</sub> based PSCs, highlighting key structural and defect properties that can be easily tuned to obtain ETL materials with purposely tailored electronic features.

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# The influence of surface treatments on the efficiency and stability of 1.68eV bandgap triple-halide perovskite solar cells

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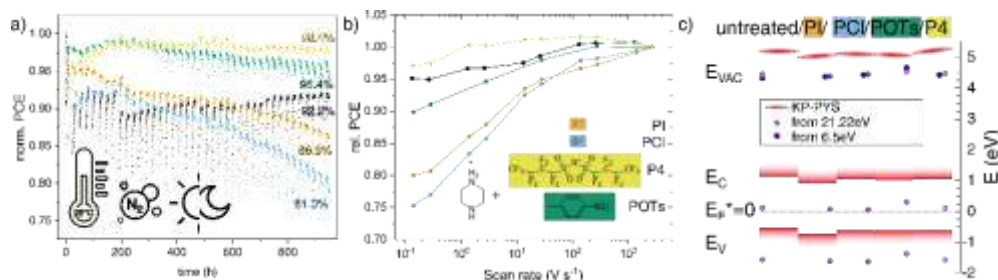
Amran Al-Ashouri,<sup>1</sup> Silvia Mariotti,<sup>1</sup> Daniele Mantione,<sup>2</sup> Sahil Shah,<sup>3</sup> Marin Rusu,<sup>1</sup> Dorothee Menzel,<sup>1</sup> Felix Lang,<sup>3</sup> Artem Musienko,<sup>1</sup> Marko Jost,<sup>4</sup> Hans Köbler,<sup>1</sup> Jinzhao Li,<sup>1</sup> David Mecerreyes,<sup>2</sup> Eva Unger,<sup>1</sup> Thomas Unold,<sup>1</sup> Antonio Abate,<sup>1</sup> Marko Topic,<sup>4</sup> Martin Stolterfoht,<sup>3</sup> Eike Köhnen,<sup>1</sup> Lars Korte,<sup>1</sup> Steve Albrecht<sup>1</sup>

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Silicon/Perovskite Tandem solar cells employing wide-bandgap (e.g. 1.68eV) perovskite absorbers demonstrated continuous improvements to a certified 32.5% efficiency in 2022 [1]. Still, to enable commercialization of this technology, the main challenge remaining is the long-term stability. In this regard, the interfaces play a crucial role due to the occurrence of electrochemical reactions, related to strong fields and charge accumulation. Post-treatment methods have been widely adopted to improve the efficiency and stability of perovskite solar cells, with a multitude of approaches [2]. Chemical passivation, field effect passivation and the reduction of energy misalignment have been identified as the main mechanisms for improvements. However, studies using model systems of interfacial modifiers with systematic variations of the molecule structure and the relation to efficiency and stability are missing. The presented work is based on the post-treatment of 1.68 eV bandgap triple-halide perovskite with a systematic variation of the anion and cation of the employed prototypical molecular salt piperazinium iodide. Piperazinium tosylate (POTs) is found to present a compromise between moderate efficiency increase and large improvements of the stability. Differences in the ionic losses (Fast-hysteresis (FH), bias assisted current extraction (BACE)) are found as the decisive factor for the initial degradation [3-4]. Additional measurements of the surface energetics (CF-SYS, KP-PYS), surface chemical environment (XPS) and near-surface structure (GIWAXS), support the hypothesis of a change in the activation energy for ion movement for the treatment with the various salts.



**Figure 1** a) Stability of cells using perovskite treated with PX (X = I, Cl, 4 (=NFSI), OTs) under ISOS-LC-1. b) Fast-hysteresis measurements of fresh devices. c) Energy diagram showing the results of Kelvin-Probe combined with Photoelectron-Yield Spectroscopy (KP-PYS), constant final state mode (CFSYS) and UPS with near-UV excitation photon energy of 6.5eV and He-UPS with excitation photon energy of 21.2eV.

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# Anharmonicity of the lead–halide bond in chlorine-substituted MAPbI<sub>3</sub> in comparison to MAPbBr<sub>3</sub>

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We report studies on three samples of chlorine-substituted MAPbI<sub>3</sub> using combined temperature-dependent synchrotron X-ray diffraction (XRD) and Pb L3-edge extended X-ray absorption fine structure (EXAFS) to analyse the bond expansion, tension effects and anharmonicity of the lead–halide bond.[1] From the results of the XRD and EXAFS analyses, the perpendicular MSD was determined, allowing a comparison of the tension and bond expansion effects in the compounds studied. In the orthorhombic phase, the positive bond expansion and the negative tension effects of the lead-halide bond were approximately equal in all three samples. However, after the transition to the disordered tetragonal/cubic phase, the balance shifted in favour of the negative tension effects in MAPbI<sub>3</sub> and MAPbI<sub>2.94</sub>Cl<sub>0.06</sub>, but in MAPbCl<sub>3</sub> the positive bond expansion seemed to predominate towards higher temperatures. The negative tension effects observed by EXAFS in the tetragonal phase of MAPbI<sub>3</sub> and MAPbI<sub>2.94</sub>Cl<sub>0.06</sub> are correlated with the behaviour of the apparent shrinking [PbX<sub>6</sub>] octahedra observed by XRD. This correlation suggests that these two compositions have stiffer Pb–X bonds and that the [PbX<sub>6</sub>] octahedra are less rigid in the tetragonal phase.

The EXAFS parameters in the orthorhombic phase were described by an Einstein or T<sup>2</sup>-type behaviour, which was then compared with the experimental EXAFS parameters of the tetragonal/cubic phase. In the orthorhombic phase, it was observed that the asymmetry of the pair distribution function (cumulant C<sub>3</sub>) is much lower in MAPbCl<sub>3</sub> than in MAPbI<sub>3</sub>. Compared to the behaviour in the orthorhombic phase, the anharmonicity changed after the phase transition to the room temperature phase, with MAPbCl<sub>3</sub> showing an increase in anharmonicity and MAPbI<sub>3</sub> showing a decrease. The differences between MAPbI<sub>3</sub> and 2% chlorine substitution were small in both the orthorhombic and tetragonal phases.

By determining the structural parameters required to convert the effective force constants  $k_0$  and  $k_3$  obtained from the EXAFS analysis into the Morse potential parameters  $\alpha$  and  $D$ , we found that our results are in agreement with other experimental results.

The results on chlorine-substituted MAPbI<sub>3</sub> are compared with results obtained by Weadock et al. in their combined EXAFS and diffraction studies on MAPbBr<sub>3</sub>.<sup>2</sup>

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# Chloride-based additive engineering for efficient and stable wide-bandgap perovskite solar cells

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Metal halide perovskite-based tandem solar cells are promising to achieve power conversion efficiency beyond the theoretical limit of their single-junction counterparts. However, overcoming the significant open-circuit voltage ( $V_{OC}$ ) deficit present in wide-bandgap (WBG) perovskite solar cells remains a major hurdle for realising efficient and stable perovskite tandem cells. The underlying material issues responsible for mediocre WBG  $V_{OC}$  include non-radiative bulk and interfacial losses,<sup>[1]</sup> light-induced halide segregation,<sup>[2]</sup> as well as heterogeneous crystallisation of the mixed-ion perovskites required for wide bandgaps.<sup>[3]</sup> Hence, effective strategies to form low-loss and stable WBG perovskites are still required.

In this study, we report a holistic approach to overcoming challenges in 1.8 eV perovskites solar cells by engineering the perovskite crystallisation pathway by means of chloride additives. In conjunction with employing a self-assembled monolayer as the hole transport layer, we achieved an  $V_{OC}$  of 1.25 V and a power conversion efficiency of 17.0%. We elucidate the key role of methylammonium chloride addition in facilitating the growth of a chloride-rich intermediate phase that directs crystallisation of the desired cubic perovskite phase, and induce more effective halide homogenisation. The as-formed 1.8 eV perovskite demonstrates suppressed halide segregation under light and improved ambient stability.

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# Chlorine Incorporation for Scalable 1.8 eV Wide Bandgap Perovskite Solar Modules with Enhanced Efficiency and Photostability

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2-terminal all-perovskite tandem solar cells have achieved certified power conversion efficiency of 29 % by combining a 1.8 eV wide bandgap with a 1.25 eV narrow bandgap perovskite solar cell. One approach to achieve a 1.8 eV wide bandgap is by alloying 40 mol% of Br in the perovskite, although this can result in low open-circuit voltage and poor photostability due to halide segregation. Moreover, the fabrication of efficient and photostable 1.8 eV perovskite polycrystalline films by scalable deposition methods over large area substrate remains a challenge.

In this contribution, we present Cl-alloyed triple halide perovskite inks for blade coating high quality perovskite absorbers with an optical bandgap of 1.8 eV, but with a Br fraction much smaller than 40 mol%. We investigate different Cl-containing precursors on their effectivity to incorporate Cl into the perovskite lattice and we identify metal-chloride as the precursor requirement to enable facile widening of the bandgap. We design various metal-chloride based perovskite precursors and evaluate their PV performance. 16 % efficient 1.8 eV perovskite solar cells with  $V_{OC}$  of 1.2 V,  $J_{SC}$  of 16.4 mA/cm<sup>2</sup> and FF of 81.1 % are achieved without interface passivation, outperforming the control sample with 40 mol% Br (**Figure 1a**). We study the photostability of these compositions and find, that CsPbCl<sub>3</sub>-alloying yields the most stable PL response over time under ~1 sun intensity (**Figure 1b**). Furthermore, we would demonstrate the scalability of our improved perovskite ink by presenting a near-infrared transparent wide bandgap perovskite solar module as well as an all-perovskite tandem module.

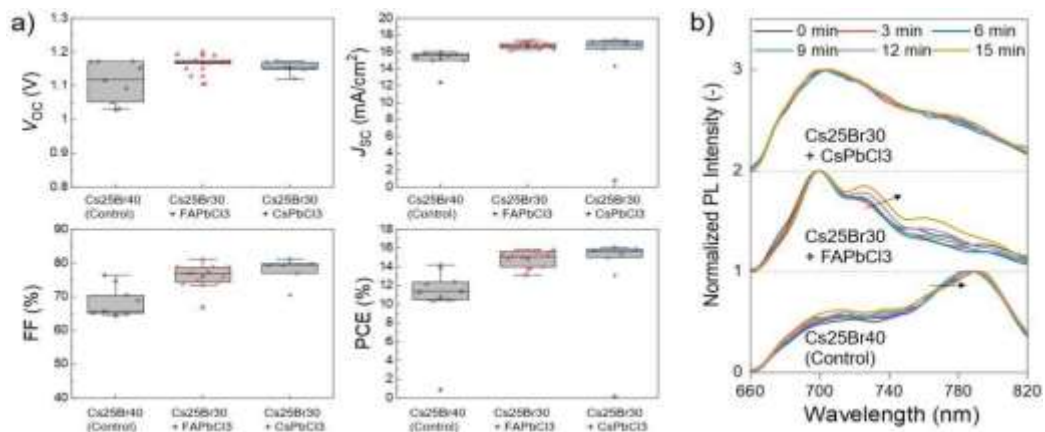


Figure 1: a) PV performance overview and b) photostability (100 mWcm<sup>-2</sup>, 640 nm) of 1.8 eV perovskite compositions: Cs<sub>0.25</sub>FA<sub>0.75</sub>Pb(I<sub>0.6</sub>Br<sub>0.4</sub>)<sub>3</sub> (Cs25Br40) compared to triple halide perovskites Cs<sub>0.25</sub>FA<sub>0.75</sub>Pb(I<sub>0.7</sub>Br<sub>0.3</sub>)<sub>3</sub> (Cs25Br30) alloyed with a metal chloride perovskite (FAPbCl<sub>3</sub>, CsPbCl<sub>3</sub>).

# Optimising sputtering conditions to fabricate SnO<sub>2</sub> films as a reliable electron transport layer for perovskite solar cell

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Perovskite solar cells (PSCs) have become popular due to rapid efficiency growth from 3.8% in 2009 to 26.08% in 2023 [1, 2]. However, to achieve commercial viability, there is a need to move away from lab-scale fabrication techniques such as spin-coating. In this project, an industrially compatible sputtering technique is investigated for fabricating the SnO<sub>2</sub> electron transport layer. The influence of several sputtering parameters such as sputtering power, film thickness, gas composition in plasma, and substrate temperature on the properties of the layer were investigated. Cell performance was then optimised sequentially to attain the maximum conversion efficiency.

The devices fabricated with lower sputtering power show a better efficiency response as lower deposition rate results in better coverage, and homogeneous SnO<sub>2</sub> films. For thickness variation, lower thicknesses of SnO<sub>2</sub> ( $\leq 20$  nm) resulted in higher open-circuit voltage and better efficiency values. The UV-vis transmission spectroscopy showed a higher transmission spectrum for smaller thicknesses of SnO<sub>2</sub> films. With varying oxygen and argon gas ratios in the sputtering chamber, the cells show a better response for higher oxygen content with maximum efficiency for 80% oxygen in the chamber. The change in oxidation states of Sn with different O<sub>2</sub>/Ar ratios in the sputtering chamber has been investigated using XPS. Further, when altering the substrate temperature during deposition, the performance of the cells increases up to 100°C but decreases with higher temperatures. The X-ray diffraction pattern of SnO<sub>2</sub> films shows higher crystalline behaviour for higher substrate temperatures. SEM and TEM will be used to further investigate the effect of substrate temperature. The best performing PSC device was obtained for 20 nm SnO<sub>2</sub> films sputtered at 100°C substrate temperature with a deposition rate of 0.058 Å/s in the sputtering chamber filled with O<sub>2</sub>/Ar (8/2) gas mixture at 2 mTorr. This best performing PSC device with optimised sputtering parameters achieved an efficiency of 11.08% as compared to 15.33% for spin-coated SnO<sub>2</sub> based devices.

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# Impact of Ion Migration on the Operational Stability of Perovskite Solar Cells: Insight from Photoemission Spectroscopy

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Despite the sky-rocketed efficiency of lead-based perovskite solar cells (PSCs) within one-decade, poor operational stability impedes the commercialization of PSCs [1]. While it is generally considered that ionic defect states in the perovskite layer inevitably lead to the degradation of PSCs, much remains unknown about the fundamental nature of ionic defects and in particular their migration in perovskite materials [2]. In this work, we utilize X-ray and Ultraviolet photoemission spectroscopy (XPS and UPS) to investigate bias dependent ion migration in PSCs. We identify that the degree of ion migration from perovskite active layer to the charge transport layers and electrode is field dependent, and is reversible, i.e., the ions that have migrated to the charge transport layer undergo back-diffusion towards the perovskite surface during storage in the dark. These spectroscopic results are correlated with the operational stability of the PSCs and expand our current understanding of ion migration in PSCs.

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# Mitigating phase segregation in co-evaporated wide band gap perovskite films for perovskite-silicon tandem application

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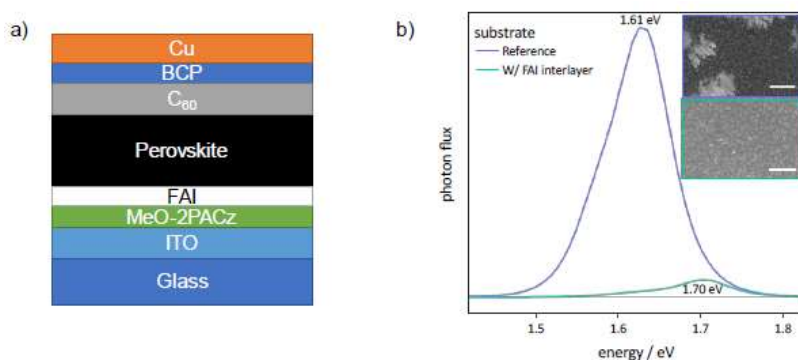
Marcel Roß,<sup>1</sup> Aleksandra Miaskiewicz,<sup>1</sup> Stefanie Severin,<sup>1</sup> Jona Kurpiers,<sup>1</sup> Lars Korte,<sup>1</sup> Steve Albrecht<sup>1,2</sup>

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In this work, we investigate phase segregation in  $\text{FA}_x\text{Cs}_y\text{Pb}_z(\text{I}_v\text{Br}_w)_3$  films obtained by co- evaporation from 4 sources, with  $\text{PbI}_2$ ,  $\text{PbBr}_2$ , formamidinium iodide (FAI) and CsI as precursors. We identify the formation of Cs-rich domains and a highly luminescent I-rich phase as the factors limiting the film quality, influencing the charge extraction, and reducing quasi-Fermi level splitting of bare films. The Cs-rich domains preferentially form at the film surface and manifest as bright clusters in scanning electron microscopy (SEM) images of the film (see inset Figure 1), while the iodide rich regions are highly luminescent in photoluminescence (PL), have a lower band gap energy compared to the film bulk and act as recombination centers, thereby lowering the quasi-Fermi level splitting and reducing open-circuit voltage ( $V_{oc}$ ) in devices [1].



**Figure 1 a)** Schematic representation of a solar cell device stack with an FAI interlayer. **b)** PL spectra of C60 covered perovskite films deposited on [2-(3,6-Dimethoxy-9H-carbazol-9-yl)ethyl]phosphonic Acid (MeO-2PACz) coated indium-tin oxide (ITO). Inset: SEM images of the corresponding perovskite films. Scale bar: 800 nm.

We show that the phase segregation is sensitive to the ratio of the precursors, substrate temperature during deposition, as well as post-deposition annealing temperature and duration. Additionally, we investigate the influence of depositing an FAI interlayer between the hole transporting layer (HTL) and perovskite (Figure 1 a), as well as a vertical compositional gradient in the perovskite film, and show how these approaches can be beneficial for the phase stability of the film. Figure 1 b) shows how using an FAI interlayer reduced the intensity of the  $\sim 1.61$  eV PL emission peak that is related to the iodine rich-phase, and prevented the formation of Cs-rich phase, as seen by the absence of bright clusters in the SEM images in the inset of Figure 1 b). With this work, we demonstrate that prevention of phase segregation leads to improved solar cell device performance for wide band gap perovskite solar cells in p-i-n architecture formed by co- evaporation, that can be utilized in perovskite/silicon tandem solar cells.

# The Impact of Surface Termination of MAPbI<sub>3</sub> Perovskite on the Electronic Structure at Interface with Rubrene

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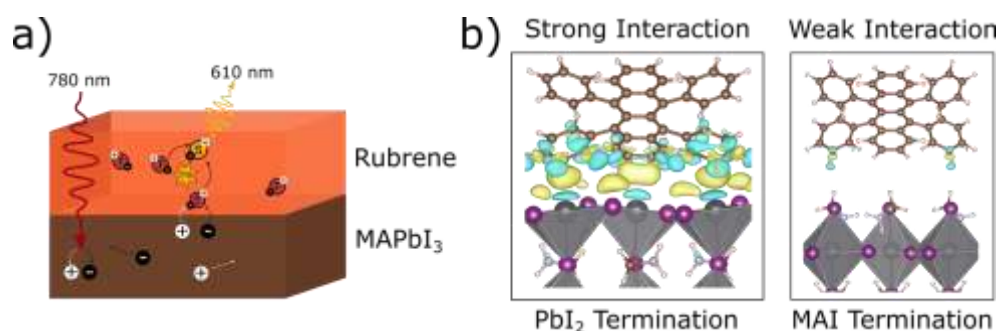
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Photon upconversion presents itself as a valuable prospect in increasing the efficiency of photovoltaics by overcoming the detailed balance limit via harvesting sub-bandgap photons [1]. Upconversion via Triplet-triplet annihilation (TTA), where two triplet (spin-1) excitons interact to become one higher energy singlet (spin-0) exciton, is of great interest due to being efficient at low powers since energy is stored in long-lived triplet excitons as recombination is spin-forbidden [1]. Whilst efficient TTA upconversion has remained elusive in the solid state, an exciting new system is based on a perovskite sensitizer with an adjacent organic-semiconductor film as an annihilator, first demonstrated in 2019 [2]. Questions remain however over how the interfacial properties of the perovskite sensitizer affect the formation of triplet excitons in the organic annihilator. In this work the electronic interaction between interfaces of rubrene and the perovskite MAPbI<sub>3</sub>, with various MAPbI<sub>3</sub> surface terminations are probed by means of density functional theory. The results show that different surface terminations of the perovskite film greatly affect the density of electrons in the supercells. Namely, for a PbI<sub>2</sub> terminated system a strong interfacial dipole ( $E_{dip} \approx 830$  meV) is formed between the MAPbI<sub>3</sub> and rubrene slabs. Contrastingly, almost no interaction is seen between a MAI terminated perovskite and rubrene, likely due to the lower density of states in the MAI layers for the rubrene to interact with. As the sensitization mechanism of triplet excitons is theorized to be via sequential charge-transfer across the perovskite/rubrene interface [2], the existence of an interfacial dipole between the sensitizer and the annihilator would have a significant impact on the efficiency of the upconverting system and presents itself as a crucial factor to control during the fabrication of these heterostructures.



**Figure 1: a) Heterostructure consisting of a MAPbI<sub>3</sub> sensitizer and rubrene annihilator.**

**b) Interfacial electron density change observed for different surface terminations of the perovskite film in the contact with rubrene.**

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# Two-step MAPbI<sub>3</sub> deposition by low-vacuum proximity-space-effusion for high-efficiency inverted semitransparent perovskite solar cells

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Halide perovskite solar cells can combine high photoconversion efficiency with high transmittance [1-3]. Herein, we describe an innovative vacuum deposition method to prepare thin CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> (MAPbI<sub>3</sub>) layers for semitransparent perovskite solar cells. The method is based on a two-step Low-Vacuum Proximity-Space-Effusion process (LV-PSE: working pressure 2–4 × 10<sup>-2</sup> mbar; source-substrate distance 1–3 cm) that guarantees high-quality of the material at low production costs. The process parameter optimization was validated by theoretical calculation. We show that during the CH<sub>3</sub>NH<sub>3</sub>I (MAI) deposition on PbI<sub>2</sub> at a given substrate temperature the conversion of the PbI<sub>2</sub> film to MAPbI<sub>3</sub> occurs from the top surface inward via an adsorption–incorporation–migration mechanism guided by the gradient of energetic MAI concentration. The quality of the final layer arises from this progressive conversion that also exploits the lattice order of the mother PbI<sub>2</sub> layer. Finally, p–i–n solar cells were prepared using ITO/PTAA/MAPbI<sub>3</sub>/PCBM-BCP/Al architectures with a photoactive layer thickness of 150 nm. This layer, characterized by an Average Visible Transmittance (AVT) as high as 20%, produced an average efficiency of 14.4% which is a remarkable result considering the transparency vs. efficiency countertrend. We demonstrated that a further down scalability of the MAPbI<sub>3</sub> layer is feasible as proved by reducing the thickness down to 80 nm. In this case, the devices showed an average efficiency of 12.9% withstanding an AVT of 32.8%. This notable efficiency recorded on those extremely thin layers thus benefits from the exclusive quality of the MAPbI<sub>3</sub> grown with the developed method[4].

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[4]E. Smecca, V. Valenzano, S. Valastro, I. Deretzis, G. Mannino, G. Malandrino, G. Accorsi, S. Colella, A. Rizzo, A. La Magna, A. Listorti, A. Alberti, J. Mater. Chem. A 2021, 9, 16456



# Characterising halide perovskite crystallisation using in situ GIWAXS

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The crystallisation pathway of metal halide perovskites from solution significantly impacts optoelectronic quality, defect formation and stability in the formed materials. While many crystalline intermediates - such as solvate and polytype phases - have been identified for typical Pb-based and I-rich compositions, much remains to be uncovered about the effect of cation, metal and halide composition on phase growth. Here we present a holistic understanding of perovskite crystallisation across a wide range of compositions and bandgaps relevant for tandem applications, and also address the role of additives in secondary phase formation.[1][2] Principally we investigate perovskite materials deposited by blade-coating and monitored using synchrotron-based in situ grazing-incidence wide-angle X-ray scattering (GIWAXS). By means of a selection of solution characterisation methods, including nuclear magnetic resonance (NMR) spectroscopy, we establish a clear understanding of the bridge between solution chemistry, precursor phase formation and resulting material properties across the entire range of PV-relevant perovskite compositions. Our work provides important insights into the controlled growth of stable perovskite materials by understanding and manipulating the crystallisation pathway.

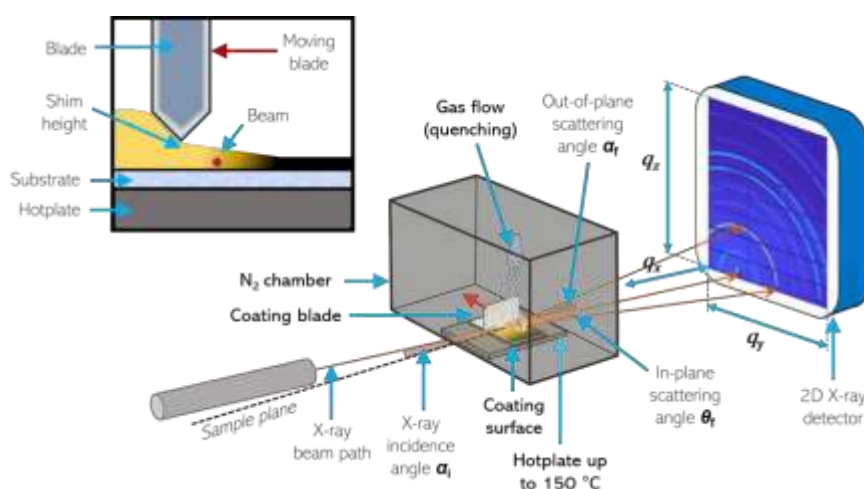


Figure 1: Synchrotron-based in situ GIWAXS on blade-coated perovskite solutions.

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# The problem of vanishing photocurrent in inorganic, wide band gap CsPbBr<sub>3</sub> perovskite solar cells

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Inorganic perovskites are known for their higher stability regard to hybrid organo- inorganic counterparts [1]. The CsPbBr<sub>3</sub> perovskite is a good example due to its structural, thermal and chemical stability that allow its deposition without necessity of using inert atmosphere and humidity control [2]. Due to the presence of cesium and even more due to bromine this perovskite is characterized by wide band gap of about

2.36 eV, which results in absorption cut off around 550 nm. Despite the band gap it might have some special application such as buildings and greenhouses or small, mobile devices. This means that the obtainable photocurrent is rather small and it is one the crucial factor that limits the solar cell efficiency. A simple calculation shows that its limit is about the 8,7 mA/cm<sup>2</sup>, therefore it is even more important to look for any possibilities to reduce the optical losses and ensure the highest possible absorption in the perovskite absorber. The investigation were done in a n-i-p configuration but in planar structure solar cells, which is quite unique for these particular perovskite. For that matter the precursor of TiO<sub>2</sub> electron transport layer was selected in order to obtain the lower refractive index contrast. By means of optical FDTD simulations the lower reflectance loses were predicted and further confirmed by UV-Vis spectroscopy, that indicated higher optical absorption in perovskite. Unexpectedly, the photocurrent obtained from the preoptimized solar cells appeared to be lower than controls. Subsequently, the initial front side FTO electrode was replaced by a new one of about twice lower thickness in order to reduce be absorption losses. Better optical performances was again confirmed by UV-Vis measurements, however the obtained photocurrent was lower once more. In both different scenarios the evidently enhanced optical absorption in perovskite led to unexpected drop of photocurrent density. In order to explain this findings we hypothesis based on AFM imaging that both a microscale and nanoscale roughness can be responsible for this phenomenon influencing the actual and effective transport of electron from perovskite to electron transport layer.

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[2] X. Li et al, *Sol. RRL* 2020, 4, 2000362.

# Industrially Compatible FAPI Perovskite Solar Cells and Modules Fabrication by Meniscus Coating Technique

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In the last decade, perovskite (pvk) solar cells (PSCs) become an hot topic for their unique optoelectronic properties and high solar energy conversion efficiency (25.7% on single junction), making them a valid alternative with respect to the well-established silicon technology [1]. Pvk strength lies in solution processes that can be scaled up with low cost and low CO<sub>2</sub> footprint fabrication methods [2,3]. The low-cost perspective of PSCs is achievable only if scalable and reliable processes in manufacturing conditions, such as pilot line or plant factory, are designed and optimized for the full device stack. Narrow bandgap pvk such as FAPI is a suitable choice to achieve good efficiency without losing stability thanks to the gap closer to the Shockley–Queisser limit. Moreover, the absence of bromine and methylammonium avoids phase segregation, widening the bandgap and thermal instability [4,5]. In this work, we show a possible route for scaling up FAPI pvk by blade coating technique in ambient environment. We explore two different FAPI sources for making pvk film, the one from precursors (PbI<sub>2</sub> + FAl) and from the one-pot synthesized powder of  $\alpha$ -phase FAPI. The pvk deposition process is based on air and green antisolvent quenching (Isopropanol, IPA) by following a recently developed method [6]. The best large area cell (0.5 cm<sup>2</sup> active area) and module (12.5 cm<sup>2</sup> active area) reached remarkable efficiency of 18.8 % and 18.4% (fig. 1), respectively. The low efficiency loss between cells and modules highlights the accuracy and the reliability of the scaling procedure for all the layers involved (SnO<sub>2</sub>/PVK/PEAI/SPIRO). Moreover, we substituted the gold counter electrode with a carbon electrode to obtain PSCs fully-printed at low temperature in ambient air.

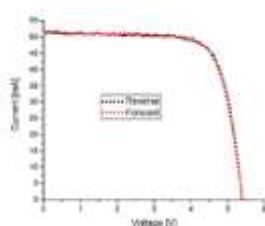


Figure 1 Mini-module IV curve.

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# Superacid treatment of metal halide perovskites to improve the absorber/hole transport layer interface

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Lewis acid-base treatments are often adopted to mitigate the effects of interfacial defects which determine the quality of heterointerfaces in perovskite solar cells (PSCs). In the case of negatively charged defects, the excess electrons of undercoordinated I<sup>-</sup> ions and Pb-I antisite defects can be passivated by a Lewis acid through coordinate bonding [1]. A typical Lewis acid, with the ability to accept pairs of nonbonding electrons, is bis(trifluoromethane)sulfonimide (TFSI). TFSI has been widely used for passivation treatment on both crystalline silicon and metal dichalcogenides, increasing the PL signal by orders of magnitude, and improving the PL quantum yield and efficiency [2].

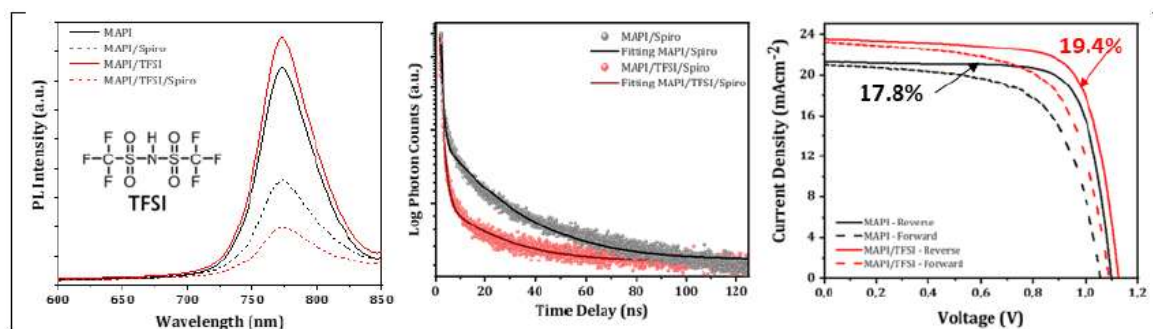


Figure 1 PL enhancement and efficiency improvement of n-i-p devices with TFSI treatment.

In the same direction, we investigate here the passivation of electron-rich surface defects in lead iodide perovskite films by TFSI. Photoluminescence spectroscopy along with transient photocurrent and photovoltage measurements proved the passivation effects of TFSI on the perovskite film, as the trap-assisted radiative electron-hole recombination was successfully suppressed and charge extraction time was decreased. XPS and UPS measurements revealed the p-type doping of the perovskite's surface and caused the vacuum level upshift, which means that charge transfer through the perovskite/HTL interface is facilitated, as charge accumulation is mitigated. As a result, TFSI treatment on perovskite surface enhanced all photovoltaic metrics compared to reference devices and the corresponding PSCs reached an improved PCE of 19.4% (Fig. 1).

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# Multi-Stage Phase-Segregation of Mixed Halide Perovskites under Illumination: A Quantitative Comparison of Experimental Observations and Thermodynamic Models

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Photo- and charge-carrier induced ion migration is a major challenge in the use of metal halide perovskite semiconductors for optoelectronic applications. Ion migration has been revealed as the underlying mechanism in most of today's instability and durability concerns in metal halide perovskites. For mixed iodide/bromide perovskites, compositional instability due to phase segregation by light or electrical bias limits the utilization of the entire bandgap region. Previous experimental and theoretical work suggests that excited states or charge-carriers trigger the process, but the exact mechanism is still controversial. To identify the mechanism and cause of the light-induced phase-segregation phenomena we investigate the full compositional range of methylammonium lead bromide/iodide samples,  $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$  with  $x = 0 \dots 1$ , by simultaneous in-situ X-ray diffraction and photoluminescence spectroscopy during illumination. Quantitative comparison of composition-dependent in situ XRD and PL shows that at excitation densities of 1 Sun, only the initial phase of photo-segregation can be explained by the previously established thermodynamic models. However, we observe a progression of the phase-segregation that can only be rationalized by considering long-lived accumulative photo-induced material alterations. We suggest that (additional) photo-induced defects, possibly halide vacancies and interstitials, must be accounted for to fully explain light-induced phase-segregation. We anticipate that our results will provide crucial insight for the development of more sophisticated models of halide phase segregation in particular, and more generally for models on the effect of photo-induced changes in material properties on ion migration.

# Surface treatment for efficient and durable formamidinium lead iodide (FAPbI<sub>3</sub>) perovskite solar cells

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Bowen Yang,<sup>1,2</sup> Anders Hagfeldt<sup>1,2</sup>

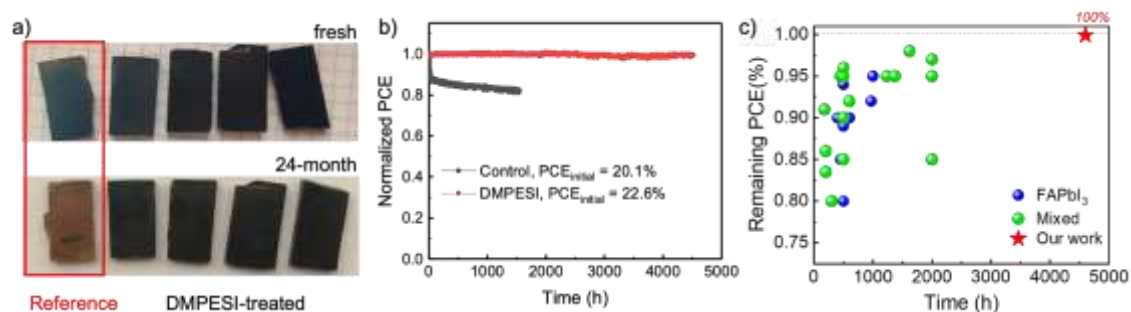
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Efficiency, stability and scalability are the most important factors on the route toward commercialization of perovskite solar cells (PSCs). Up till now, both efficiency and scalability of the PSCs have been successfully managed to comparable with the commercially used Si based solar cells. Although stability has also been significantly improved, it still remains the most critical limitation for commercializing state-of-the-art highly efficient perovskite-based photovoltaics and further improvement is critically required.

In my recent work, various novel surface passivation materials were designed and employed, to stabilize grain boundaries and surfaces of the formamidinium lead iodide (FAPbI<sub>3</sub>) based perovskite layer. The most effective passivation material shows outstanding stability upon light soaking and remarkably remains in black-phase after 2 years ageing under ambient condition without encapsulation (**Fig 1a**). The treated PSCs deliver an excellent operational stability of highly-efficient PSCs with less than 1% performance loss after more than 4500 h at maximum power point tracking, yielding an extraordinarily high theoretical  $T_{80}$  of over 9 years under continuous 1-sun illumination (**Fig 1b**). As shown in **Fig 1c**, our surface passivated device is one of the most stable PSCs reported so far.



**Fig (a)** Pictures of perovskite films before and after 24 months in ambient air. **(b)** Long-term operational stability of the unencapsulated cells under MPPT with continuous one sun illumination. **(c)** Operational stability of state-of-the-art highly efficient (PCE>22%) PSCs summarized from literature.

# Interpreting Halide Perovskite Semiconductor Photoluminescence Kinetics

Margherita Taddei

Sarthak Jariwala, Robert J. E. Westbrook, Shaun Gallagher, Aaron Weaver, Mark E. Ziffer, Jian Wang, Henry J. Snaith, David S. Ginger

**Abstract:** Drawing from both experimental data and simulation, we highlight best practices for fitting time-resolved photoluminescence (TRPL) decays on halide perovskite semiconductors now widely studied for applications in photovoltaics and light-emitting-diodes (LEDs). We focus on three key observations. First, at low excitation intensities, high-quality perovskites often show pseudo-first-order kinetics, consistent with classic minority carrier lifetimes. Second, non-single-exponential decays frequently observed at low excitation intensity often have significant contributions from spatial heterogeneity. We recommend fitting such decays by stretched exponentials, where the stretching factor ( $\beta$ ) can be used to characterize the heterogeneity of the local lifetime distribution. Third, PL decay kinetics can depend on the excitation wavelength. We discuss how penetration depth, carrier diffusion, and surface recombination affect measurements, and make recommendations for choosing experimental parameters suited to the question at hand. Accounting for these factors will provide more reliable and physical interpretation of carrier recombination and better understanding of non-radiative losses in perovskite semiconductors.

# 3D/2D heterojunction for efficient and stable perovskite solar cells based on chemical bath deposition SnO<sub>2</sub> electron transport layers

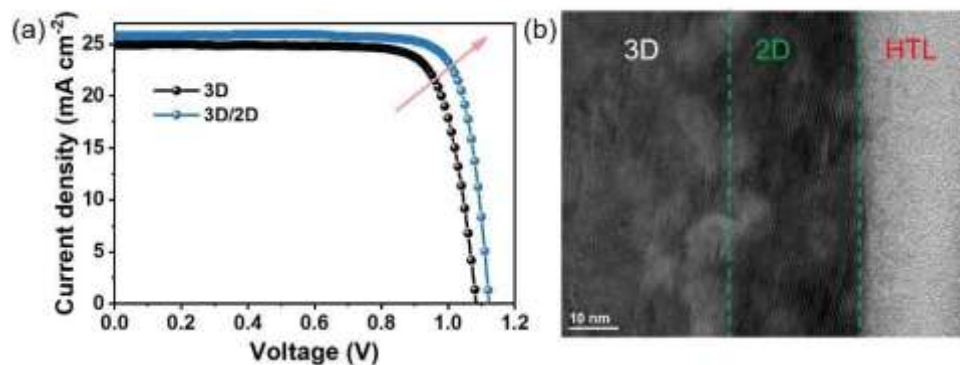
Shun Tian<sup>1</sup>

Xiaoxin Gao,<sup>1\*</sup> Mohammad Khaja Nazeeruddin,<sup>1\*</sup> Paul Joseph Dyson<sup>1\*</sup>

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Chemical bath deposition (CBD) technique has been demonstrated to yield high-quality SnO<sub>2</sub> electron transport layers (ETLs) for efficient perovskite solar cells (PSCs) [1,2]. First, high-quality SnO<sub>2</sub> films with low oxygen vacancies and good energy level alignment relative to the perovskite layer was obtained by controlling CBD time. Second, a novel alkylammonium salt spin-coated on 3D perovskites was used to create a 3D/2D heterojunction. The 3D/2D heterojunction enhances the power conversion efficiency (PCE) of PSCs from 21.39% (3D device) to 23.70% (3D/2D device) by passivating defects [3,4] and promoting charge carrier extraction [4,5] (Figure 1). Furthermore, the thermal and humidity stability of the PSCs were significantly improved because of the hydrophobic 2D perovskite surface and impeding ion migration.



**Figure 1. (a) Current density-voltage curves of PSCs. (b) High-resolution TEM image of 3D/2D perovskite heterojunction.**

[1] Yoo J. J., Seo G., Chua M. R., Park T. G., Lu Y., et al. *Nature* (2021), 590, 587-593.

[2] Park J., Kim J., Yun H. S., Paik M. J., Noh, E., et al. *Nature* (2023), 616, 724-730. [3] Jiang Q., Zhao Y., Zhang X. Y., Yang X. L., Chen Y., et al. *Nature Photonics* (2019) 13, 460-466.

[4] Azmi R., Ugur E., Seitkhan A., Aljamaan F., Subbiah A. S., et al. *Science* (2022) 376, 73-77.

[5] Du Y., Tian Q., Wang S., Yang, T., Yin, L., et al. *Advanced Materials* (2023) 35, 2206451.



# **Encapsulation and Stability of Emerging Photovoltaic Technologies Outdoors in the UK**

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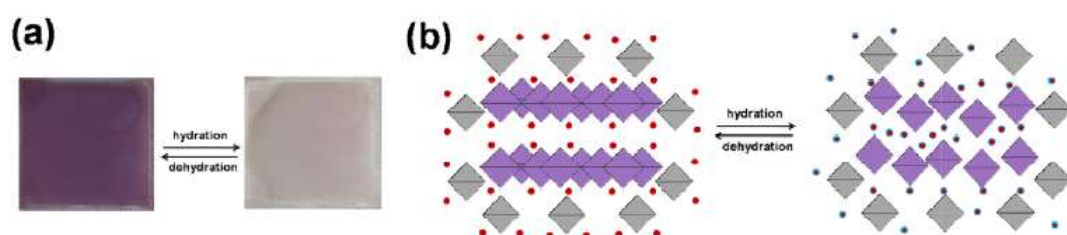
Emerging photovoltaic (PV) technologies such as halide perovskite and dye-sensitised solar cells offer unique advantages and potentials with regards to meeting UK's Net Zero target, owing to its low-cost manufacture estimate, solution processability, and non-dependence of natural resources and minerals from a few if not one single country. However, stability issues against extrinsic and intrinsic factors of working solar cells and modules hamper entry of emerging PV to mass production lines. So past few years have seen larger investment of time and funding to improve stability by encapsulation and accelerated aging the cells with artificial conditions using climate chambers or home-made set up. Outdoor stability tests in the other hand provide a greater confidence and larger relevance with respect to country-specific climate. Here, we will share our recent encapsulation efforts followed by outdoor tests in Northeast of England using bespoke testing rig developed at Newcastle University, under ViTAL Living Lab project. The main aim of the ViTAL Living Lab project is to assist our funder, Royal Air Force, in making evidence-based policy with regards to decarbonising electricity and heating to achieve RAF's Net Zero targets in 2040 by looking at potentials of emerging PV technologies in UK's cloudy climate that have not been investigated so far

# Vacancy Ordered Double Perovskite Caged 2D- Light Absorbing Perovskite for Optical Humidity Sensing

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Maintaining humidity level below 70% RH prevents molds, mites, bacteria, viruses and fungal growth in homes. Moreover, it also mitigates the risk of allergic rhinitis and asthma [1,2]. Dehumidifiers condense moisture from the atmosphere continuously to regulate the high level of humidity. In this process, they consume high amount of energy. This amount could be significantly reduced if the instrument could turn itself off after achieving certain level of humidity. Herein, we prepare an optical humidity sensor based on lead-free halide perovskite with a cut-off above 70% RH. Caging a light absorbing 2D-perovskite under a network of vacancy ordered double perovskite (VODP) allowed the composite to be used for optical humidity sensing. Unlike pure VODP, this resulting material absorbs light in the visible region with peak maximum centered on 510 nm. The film of this material changes color upon being subjected to humidity. This phenomenon was studied via in-situ XRD, in-situ UV-Vis Transmittance and Scanning Electron Microscopy. The roles of each of the phases were studied using the in-situ XRD. The dissolution of crystalline 2D-perovskite (caged inside a network of permeable VODP) into amorphous perovskite phase leads the optical color change. The device works linearly with two different rates in the ranges 10-60% RH and 70-90% RH. The device is exceptional in performance with respect to the available 2D-perovskite based optical humidity sensor. It possesses negligible hysteresis, fast response and recovery times, and high reproducibility. Additionally, the 50-fold increase in the device's transmittance rate in the range 70 - 90% RH makes the material an ideal candidate for hygrometers.



**Figure 1 (a) Image of the film at 40% RH (left) and 90% RH (right). (b) Graphical representation of the conversion of 2D-perovskite (purple colored film) to amorphous form (colorless film) on hydration. The 2D-perovskite is caged under a permeable matrix of VODP.**

[1]Thammanoon Sookchaiya, Veerapol Monyakul, and Sirichai Thepa, *Proceedings of the EDU-COM 2008 International Conference* (2008), 505-513.  
[2]A. Baughman, and Arens. E. *ASHRAE Transactions* (1996),102 (1),193-211.

## 2d/3d Perovskite Heterojunction Solar Cells: Pairing Performance With Stability

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Metal halide perovskite has become an attractive class of material for the photovoltaic (PV) industry, thanks to promising results obtained by lab-scaled devices. However, the lack of stability still hinders the early commercialization of this technology. A widely adopted method to improve the device lifetime relies on reducing the defect density in the perovskite. Defects have been proved to be one of the major causes of performance losses over time.[1] Therefore, defects passivation is a powerful strategy not only to suppress charges recombination but also to enhance the operational lifetime of the device. In particular, the insertion of two dimensional (2D) perovskite layers in between the three dimensional (3D) bulk perovskite and adjacent transport layers is a powerful approach to reduce the defects at the surface and improving simultaneously the device stability. These benefits are also supported by enhanced thermal stability of the 2D perovskite, and better resilience against environmental agents.[2] However, this approach is limited to the realization of a single 2D/3D heterostructure atop of the perovskite layer. Here, we extended this approach realizing a double 2D/3D heterostructure, passivating the top and bottom surface of the perovskite film at once. The heterostructure is formed by the conversion of the 3D phase into the 2D phase. This conversion is significantly complicated at the bottom surface. Here, the 2D precursors must be deposited on the substrate prior to the perovskite film, with a relatively higher concentration than for top conversion. Indeed, a large part of the ligands are washed away during the perovskite deposition process, while a small fraction is incorporated in the solvate film. In this work, we test different solution-based deposition methodologies which allow to create the double 2D/3D heterostructures and we evaluate the device performances from a list of different cations, emphasizing both enhanced performances and stability.

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[1]E. Aydin, M. De Bastiani and S. De Wolf, *Advance Materials* (2019), 31(25)

[2]R. Azmi, E. Ugur, A. Seitkhan et al., *Science* (2022), 73-77,376(6588).

# Driving Lattice Dynamics in 2D Perovskites via THz Kerr Effect

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Charge carrier-phonon interaction governs the majority of lead halide perovskite's optoelectronic properties. Understanding their complex vibrational dynamics and microscopic coupling mechanisms is crucial for improved material design. Recently, we used intense single-cycle THz pulses to coherently drive octahedral twist modes, providing a handle to study and control the perovskite crystal lattice [1].

Layered hybrid organic-inorganic perovskites (HOIPs) combine the intriguing HOIP properties originating from the soft, polar, and anharmonic lattice with confinement effects arising from the reduced dimensionality. Here, we study layered Ruddlesden-Popper HOIP compounds  $(\text{PEA})_2(\text{MA})_{n-1}\text{Pb}_n\text{I}_{3n+1}$  with  $n = 1, 2, 3$ . We drive the lattice using sub-picosecond THz electric field pulses and observe the ensuing dynamics by probing the transient pump-induced birefringence (THz-induced Kerr effect). In contrast to 3D HOIPs, already at room temperature we observe long-lived oscillations in the 0.5–3 THz range due to the modulation of lattice polarizability by nonlinearly driven Raman-active modes. We analyze the mode symmetry and driving mechanisms based on the  $\chi^{(3)}$  effective nonlinear susceptibility tensor formalism. Comparing the dynamics for different  $n$ , we identify a unique 3 THz mode, which is likely governed by the presence of the PEA organic layer.

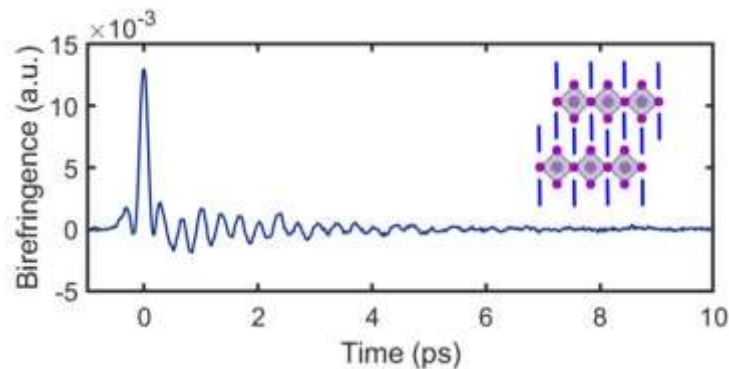


Figure 1 THz-induced birefringence in  $(\text{PEA})_2\text{PbI}_4$ .

*Our work constitutes a step towards a better understanding of phonons in lower dimensional HOIPs and their contribution to exciton self-trapping, charge carrier screening or dynamic symmetry breaking.*

[1]M. Frenzel, M. Cherasse et al., arXiv:2301.03508 [cond-mat.mtrl-sci] (2023)

# Synergistic approach towards enhanced stability and emission of FAPbBr<sub>3</sub> NCs for LED applications

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As the global population continues to grow, the pursuit of efficient and sustainable lighting solutions remains an indispensable endeavor. Perovskites promise a bright future for next-generation light-emitting diodes (LEDs), as these materials allow facile and cheap solution processing, while exhibiting easily tuneable bandgaps, high color purity, high photoluminescence quantum yields (PLQY), and impressive external quantum efficiencies (EQE).

Unfortunately, there are still a few major hurdles to overcome before commercializing perovskite-based LEDs. First, their operational stability is inferior to current market standards. Secondly, blue LEDs have a much lower efficiency than their green and red counterparts.

In this poster, I will present two closely related projects. The first one concerns our recently published work [1]. Here we succeeded in greatly increasing the stability of green-emitting FAPbBr<sub>3</sub> nanocrystals (NCs) under humid conditions with PLQYs reaching near unity. This was made possible through a synergistic approach that combined additive engineering with the development of a suitable post-treatment. Eventually, their use in LEDs was demonstrated [1].

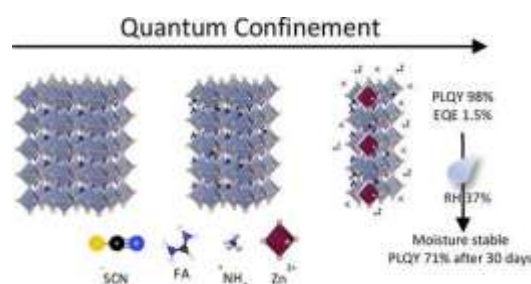


Figure 1 Schematic representation of the main takeaways of [1].

Building on the success of the previous work, we are currently leveraging the insights gained throughout this project to push the boundaries even more and extend the scope toward blue-emitting LEDs. By making further modifications to these FAPbBr<sub>3</sub> NCs, strongly emissive sky-blue NCs were obtained. The promising preliminary results along with some mechanistic insights will also be presented.

*These projects offer a significant step forward in advancing perovskite-based LEDs, moving us closer to achieving highly efficient and stable lighting solutions for a sustainable future.*

[1] H. Bhatia, L. Van Gaal, E. Debroye\* et al. *ACS Applied Optical Materials* (2023), 1,6, 1184-1191.

# Tailoring Interlayer Charge Transfer Dynamics in 2D Perovskites with electroactive ligands

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Yorrick Boeije,<sup>2,3</sup> Youcheng Zhang,<sup>3,4</sup> Pratyush Ghosh,<sup>3</sup> Szymon J. Zelewski,<sup>2,3</sup> Arthur Maufort,<sup>1</sup> Bart Roose,<sup>2</sup> Zher Ying Ooi,<sup>2</sup> Rituparno Chowdhury,<sup>3</sup> Ilan Devroey,<sup>1</sup> Stijn Lenaers,<sup>2</sup> Alasdair Tew,<sup>3</sup> Linjie Dai,<sup>2,3</sup> Krishanu Dey,<sup>3</sup> Hayden Salway,<sup>2</sup> Richard H. Friend,<sup>3</sup> Henning Sirringhaus,<sup>3</sup> Laurence Lutsen,<sup>1,5</sup> Akshay Rao,<sup>3</sup> Samuel D. Stranks,<sup>2,3</sup> Dirk Vanderzande,<sup>5</sup>

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The family of hybrid organic-inorganic lead-halide perovskites are the subject of intense interest for optoelectronic applications. Due to the inert nature of most organic molecules, the inorganic sublattice generally dominates the electronic structure and therefore optoelectronic properties of perovskites. We use optically and electronically active carbazole-based Cz-Ci molecules[1-2], where Ci indicates an alkylammonium chain and i indicates the number of CH<sub>2</sub> units in the chain, varying from 3–5, as cations in the 2D perovskite structure (Cz-Ci)<sub>2</sub>PbI<sub>4</sub>. We demonstrate a tunable electronic coupling between the inorganic lead-halide and organic layers. The strongest interlayer electronic coupling was found for (Cz-C3)<sub>2</sub>PbI<sub>4</sub>. We measure ultrafast hole transfer from the photoexcited lead-halide layer to the Cz-Ci molecules, the efficiency of which increases by varying the chain length from i=5 to i=3. The charge transfer results in long-lived carriers (10–100 ns) and quenched emission. Electrical charge transport measurements show increased out-of-plane carrier mobility compared to PEA, with carrier mobility increasing from i=5 to i=3.[3]

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[1]Herckens, R.; Van Gompel, W. T. M.; Song, W. Y.; Gelvez-Rueda, M. C.; Maufort, A.; Ruttens, B.; D'Haen, J.; Grozema, F. C.; Aernouts, T.; Lutsen, L.; Vanderzande, D., *Journal of Materials Chemistry A* 2018, 6 (45), 22899-22908 (10.1039/c8ta08019d)

[2]Van Landeghem, M.; Van Gompel, W. T. M.; Herckens, R.; Lutsen, L.; Vanderzande, D.; Van Doorslaer, S.; Goovaerts, E., *The Journal of Physical Chemistry C* 2021, 125 (33), 18317-18327 (10.1021/acs.jpcc.1c05005)

[3]Boeije, Y.; Van Gompel, W. T. M.; Zhang, Y.; Ghosh, P.; Zelewski, S.; Maufort, A.; Roose, B.; Ying Ooi, Z.; Chowdhury, R.; Devroey, I.; Lenaers, S.; Tew, A.; Dai, L.; Dey, K.; Salway, H.; Friend, R. H.; Sirringhaus, H.; Lutsen, L.; Vanderzande, D.; Rao, A.; Stranks, S. D., *Journal of the American Chemical Society* 2023, Just Accepted (10.1021/jacs.3c05974)

# Light dependency for current - voltage curve hysteresis in perovskite solar cells modelled by slow - shallow trap states

W. Veurman

J. Kern, M. Müller, R. Peibst, F. Haase and S. Kajari Schröder

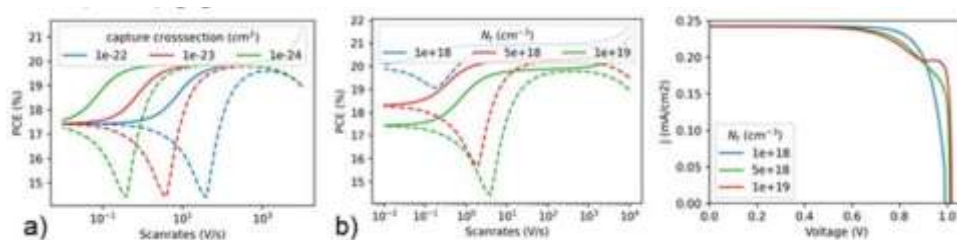
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Device modelling shows that a hysteresis of the current-voltage curve as caused by slow-shallow-trap-states (SSTs) is to a large extent equivalent to the assumption of moving ions in the perovskite. A difference arises for the illumination dependence of the hysteresis. This offers an opportunity for experimentally distinguishing between the two explanatory models.

Hysteresis in current-voltage measurements is a typical phenomenon seen in perovskite solar cells (PSC) at higher scan speeds. A maximum hysteresis effect is present for medium scan speeds, compared to low or very fast scan speeds [1]. The height of this maximum can be seen as a measure for the PSC quality, where more efficient and more stable cells tend to show a smaller hysteresis. The effect of hysteresis has been explained by moving ion vacancies through the perovskite bulk. Another explanation that has been suggested is the occurrence of shallow defect states in the perovskite near the transport layers, with very small captures cross-sections, so-called “slow-shallow- trap-states” (SSTs) [2].



**Figure 1** Power conversion efficiency at different scan speeds, for measurement from  $V_{oc}$  to  $J_{sc}$  (solid lines) and back (dashed lines), for different  $N_t$ 's (a) and various capture cross-sections (b). I-V curves at 0.01 sun, scan-rate 630 V/s and various  $N_t$ 's (c).

We have developed a complete device model, using the Sentaurus™ Device software from Synopsis. By incorporating SSTs within the model, we can reproduce the hysteresis maximum at medium scan speeds depending on the local trap density ( $N_t$ ) or their capture cross-section (fig.1a-b). We find the two models, “ion-movement” versus “SSTs” to be equivalent in many aspects. However, when analysing the light dependency of the hysteresis effect within the two explanatory frameworks, differences arise, which could be used to experimentally distinguish between the two models. For example, a capacitive effect arises for the SST-model at higher scan speeds and lower light intensities (fig. 1c), when the number of traps in the model increases.

[1] V.M. Le Corre, J. Diekmann, H.J. Snaith, D. Neher, M. Stollerfoht, *Solar RRL* (2022), 6(4).

[2] R. van Heerden, P. Procel, L. Mazzarella, R. Santbergen O. Isabella, *Front. Photonics* (2022), 3:889837.

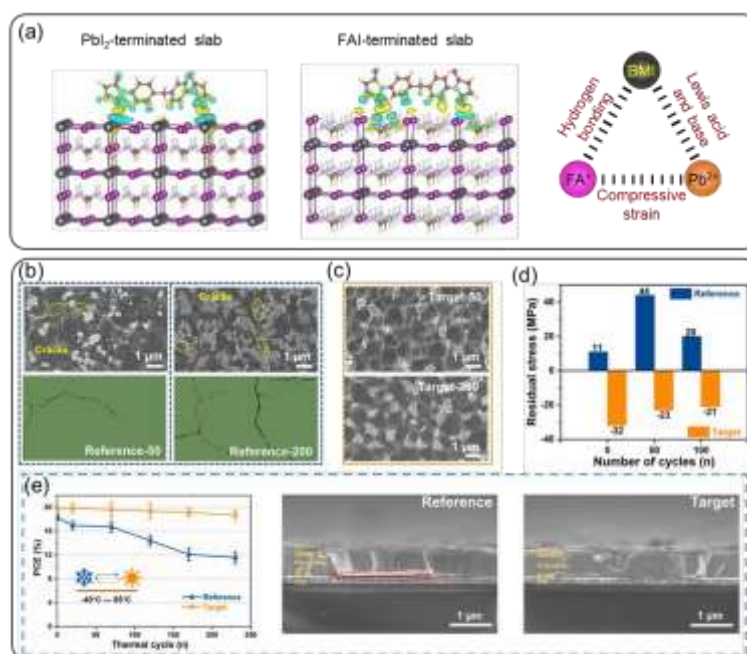
# Stabilizing Perovskite Solar Cells via Compressive Strain

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Metal halide perovskites are promising as next-generation photovoltaic materials, but stability issues are still a huge obstacle to their commercialization. Stabilizing formamidinium (FA)-based perovskite through compressive strain is reported. The 1,1'(methylenedi-4,1-phenylene) bismaleimide (BMI) was introduced to toughen the perovskite interface. The chemical bonding and strain modulation synergistically not only passivate film defects and inhibit perovskite decomposition[1]. The formation and evolution of cracks in perovskite films during thermal cycling, which affect their stability, are investigated. Compressive strain is employed to suppress cracks and delamination by in situ formed polymers with low elastic modulus during crystal growth. The resultant devices retain 95% of the initial power conversion efficiency (PCE) and compressive strain after 230 cycles[2]. Those findings shed light on strain engineering with respect to their evolution, which enables stable perovskite solar cells.



**Figure 1 Compressive strain enhanced stability.** (a) DFT calculations of charge difference between BMI and FAPbI<sub>3</sub> and schematic mechanisms of a stable triangle structure to reinforce the stability of FAPbI<sub>3</sub>. SEM images of the Reference perovskite films (b) and Target perovskite films (c) at 50 and 200 cycles. (d) Residual stress values of the Reference and Target perovskite films after 0, 50, and 100 thermal cycles. (e) Thermal cycle stability (−40 to 85 °C, ramp rate of 100 °C h<sup>−1</sup>) of encapsulated perovskite solar cells and cross-sectional SEM images of the devices after the thermal cycle.

[1]Shi C. et al. *Adv. Funct. Mater.* (2022), 32, 2201193.

[2]Yuan G. et al. *Adv. Mater.* (2023), 35, 2211257.



## **Mastering the crystallization dynamic of FAPbI<sub>3</sub> thin film for high efficiency and stable light-emitting diodes.**

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Formamidinium lead iodide (FAPbI<sub>3</sub>) perovskite semiconductor has been widely used for solar cells, light-emitting diodes (LEDs), detectors, lasers, etc. However, the growing strategies of FAPbI<sub>3</sub> polycrystalline thin films are different when they are embodied in different optoelectronic devices, despite common needs of achieving phase stability and high photoluminescence quantum yields – one of the most common figures of merit to optimize a semiconductor thin film. Here, we investigate the growing strategies for FAPbI<sub>3</sub> thin films for LED applications. We show how the crystallization dynamic as a function of the precursors and additive engineering determine the presence of point defects, strain, and “impurities” in the deposited FAPbI<sub>3</sub> thin films. By mastering the crystallization process and the components of the deposited “FAPbI<sub>3</sub>” thin film, we demonstrated high-efficiency (24.5%) and stable (LT<sub>90</sub>=147h, at constant current density of 20 mA cm<sup>-2</sup>) LEDs.

# Device Physics of Ion-defect-coupled Perovskite LEDs

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Due to the exceptional chemical versatility and superior optoelectronic features, halide perovskites are anticipated to emerge as promising candidates for next-generation semiconductor applications. Nonetheless, uncontrollable ion migration remains a critical challenge, impeding their path towards commercialization. This issue is particularly pronounced in perovskite LEDs, where strong electric fields can induce significant migration of these charges. While attempts have been made to elucidate and explore the migration mechanisms in perovskite materials, limited studies have addressed these physical processes within the device itself, especially thin LEDs.

Mobile ions demonstrate diffusion and drift behaviors under the influence of concentration gradients and electric fields, respectively, but cannot be externally replenished through electrical circuits, in contrast to charged carriers (i.e., electrons and holes). Meanwhile, these charges will substantially impact each other and alter carrier distributions in the perovskite layer. More importantly, the complex coupling also includes the defect-controlled carrier dynamics and ion-defect coupling, which cannot be elucidated as the sum of carrier dynamics and ion migration.

In this work, we realized the coupling of ion migration and defects to examine the influence of these extra charges on the device performance as mobile charges and defect passivators. Our findings reveal a strong correlation between ion and carrier distributions, in which an increased presence of mobile ions within the perovskite layer changes the recombination profiles in the active layer considerably, as illustrated in the accompanying figure. This theoretical investigation reveals the significance of ion migration and emphasizes the possible utilization of mobile ions in the perovskite LEDs for high efficiency and stability and future development of lasing devices.

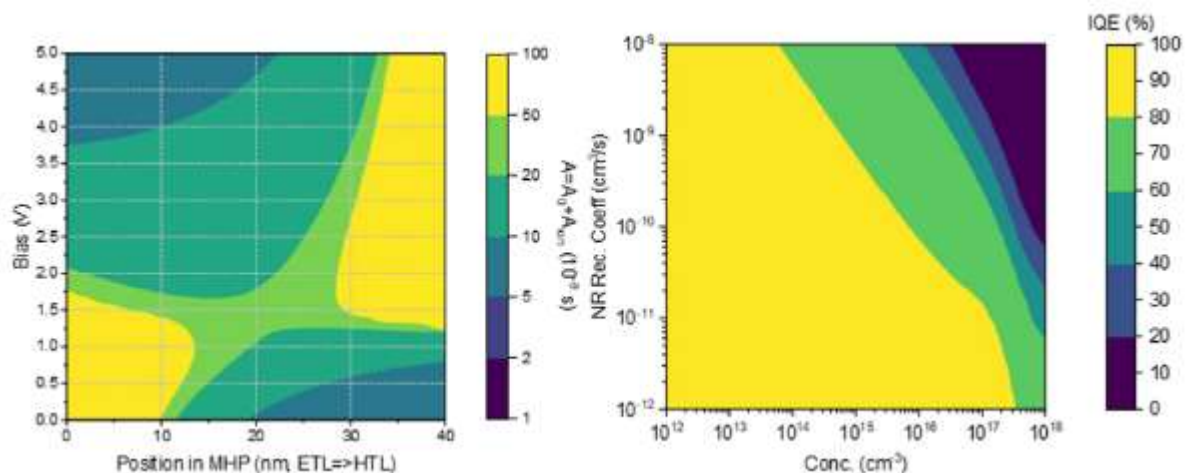


Figure 1 a) Ion-coupled SRH Recombination profile in the operation devices. b) IQE distribution of ion-defect non-radiation and ion density.

# Vacancy-mediated Cs<sup>+</sup> and Br<sup>-</sup> ion migration in biaxially strained CsPbBr<sub>3</sub>

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<sup>1</sup>Department of Chemistry – Ångström Laboratory, Uppsala University, Sweden.

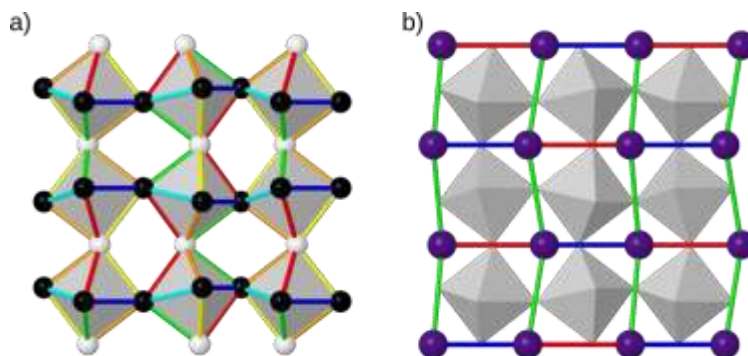
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The instability of halide-perovskite-based devices is exacerbated by the tensile strain resulting from post deposition thermal treatments [1,2]. The effects of strain on stability have been attributed to changes in the activation barriers for ionic migration, and there exists computational evidence that anion migration barriers are lowered by tensile strain and raised by compressive strain [3], but a thorough atomistic analysis of this interplay is currently lacking, and cation migration has not been considered.

I will present the results of our study of the effects of biaxial strain on vacancy-mediated Cs<sup>+</sup> and Br<sup>-</sup> ion migration in CsPbBr<sub>3</sub>, following on from our recent paper on the effects of hydrostatic pressure [3]. We used DFT to calculate the activation barriers for ions to hop between all of the symmetrically inequivalent nearest-neighbour pairs of lattice sites (see Figure 1), and used the resulting values to calculate diffusion coefficient tensors from kinetic theory. Isotropic biaxial strains in the (001), (010) and (100) planes in the range -5% to +5% were considered. The main result is that Cs<sup>+</sup> migration is significantly more strongly affected by biaxial strain than Br<sup>-</sup> migration, and can differ by several orders of magnitude between strain states. This result suggests that the strong dependence of perovskite device stability on strain might be due to A-site cation migration, rather than anion migration, in contrast to common assumption.



**Figure 1** Structure of the orthorhombic Pnma phase of CsPbBr<sub>3</sub>, showing the connectivity of (a) the Br<sup>-</sup> (black/white spheres) and (b) the Cs<sup>+</sup> (purple spheres) sub-lattices. Pairs of ions are connected by sticks coloured according to their symmetric equivalence.

[1] Q. Tu, D. Kim, M. Shyikh and M. G. Kanatzidis, *Matter* (2021), 4, pp 2765–2809.

[2] D. Liu *et al.*, *Nat. Mater.* (2021), 20, pp 1337–1346.

[3] D.-J. Xue *et al.*, *Nat. Commun.* (2021), 11, 1514.

[4] T. J. A. M. Smolders, A. B. Walker and M. J. Wolf, *J. Phys. Chem. Lett.* (2021), 12, pp 5169–5177.

# The influences of excess FAI to ASE performances and carrier dynamics in FAPbI<sub>3</sub> perovskite

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The utilization of excessive formamidinium iodide (FAI) in formamidinium lead iodide (FAPbI<sub>3</sub>) has long been employed as a conventional strategy to enhance the efficiency of light-emitting diodes (LEDs) <sup>[1,2]</sup>. However, until now, the effects of excess FAI on amplified spontaneous emission (ASE) performances and carrier dynamics in the FAPbI<sub>3</sub> system have remained unexplored.

In this study, we discovered that the presence of excessive FAI enhances the photoluminescence quantum efficiency (PLQY). This improvement in PLQY can be attributed to the induction of carrier transfer from the low dimensional phase of the perovskite material, revealing a new mechanism by which excess FAI can positively impact the system's performance.

Surprisingly, it was observed that the ASE threshold increases with the addition of excess FAI, contrary to our initial expectations. This counterintuitive result suggests that the interplay between FAI concentration and the stimulated emission process is more intricate than previously thought, requiring a deeper understanding of the underlying dynamics.

We employed a fundamental three-level laser rate equation model <sup>[3]</sup>, and ultrafast transient absorption spectroscopy. Through these techniques, we were able to explain the interplay between FAI concentration, photoluminescence quantum efficiency, and ASE, providing valuable insights into the effects of this conventional trap engineering strategy in a different direction.

This study provides a more straight forward way to help us understanding the difference focus point between choosing the perovskite material as a laser gain media and LED active layer material.

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[1]Jia, Y. H., S. Neutzner, et al. Adv. Funct. Mater (2019) **30**(1).

[2]Wang, H., F. U. Kosasih, et al Nat Commun (2020) **11**(1): 891.

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# Carrier–Phonon Interaction Induced Negative Thermal-Optic Coefficient at Near Band Edge of Quasi-2D (PEA)<sub>2</sub>PbBr<sub>4</sub> Perovskite

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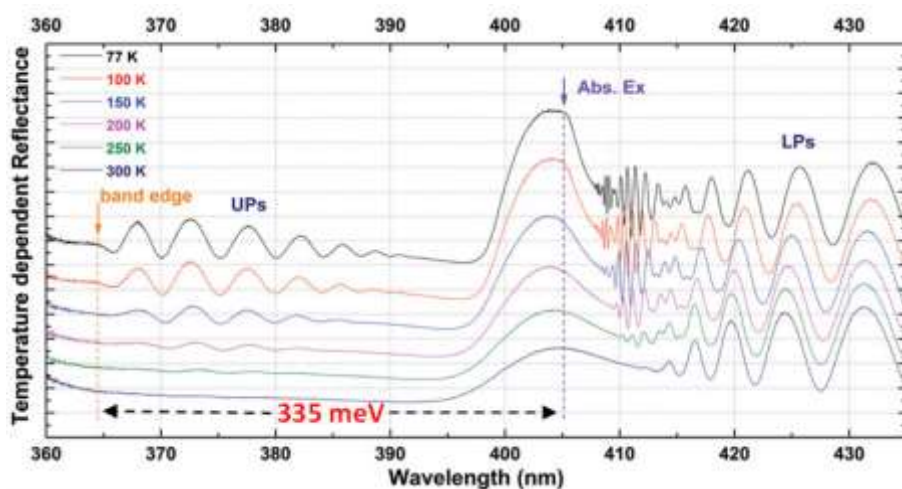
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We studied the optical resonant modes in temperature-dependent (77 K to RT) spectroscopy and investigated the effect of the quasi-particles (exciton-polariton- polaron) on refractive index dispersion. The large binding energy (about 335 meV) of quasi-2D excitons is obtained by the reflectance measurements at 77 K. Stable exciton- polaritons and exciton-polarons are proved by energy dispersions and the self-trapped exciton-polaron state [1]. Furthermore, the large negative thermal-optic coefficient due to the damping effect of exciton-phonon scattering is confirmed. This phenomenon is opposite to those observed in conventional semiconductors (e.g., Si, Ge, GaN, GaAs, ZnO, etc.). In addition, the observation of stable negative thermal-optic coefficients from 160 K to RT suggests that the quasi-2D (PEA)<sub>2</sub>PbBr<sub>4</sub> perovskite can be adopted as a phase compensator for conventional semiconductor materials [2].



**Figure 1.** Temperature-dependent reflectance spectra of (PEA)<sub>2</sub>PbBr<sub>4</sub>. The “UPs” and “LPs” indicate the upper polariton and lower polariton branches, respectively. The “Abs. Ex” is the estimated exciton energy level. The binding energy is about 335 meV and the “band edge” means the continuous band edge.

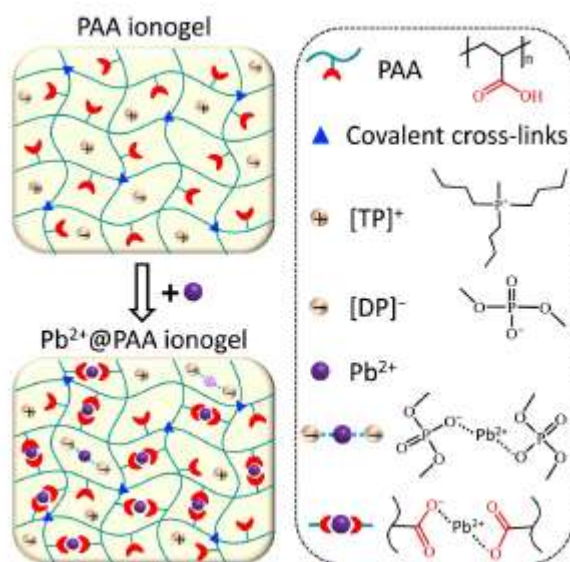
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# Lead-Absorbing ionogel-based encapsulation for impact-resistant, stable, and lead-safe perovskite modules

Xun Xiao

Despite the high-efficiency and low-cost prospect for perovskite solar cells, great concerns of lead toxicity and instability remain for this technology. Here, we report an encapsulation strategy for perovskite modules based on lead-adsorbing ionogel, which prevents lead leakage and withstand long-term stability tests. The ionogel layers integrated on both sides of modules enhance impact resistance. The self-healable ionogel can prevent water permeation into the perovskite layer and adsorb lead that might leak. The encapsulated devices pass the damp heat and thermal cycling accelerated stability tests according to International Electrotechnical Commission 61215 standard. The ionogel encapsulation reduces lead leakage to undetectable level after the hail-damaged module is soaked in water for 24 hours. Even being rolled over by a car followed by water soaking for 45 days, the ionogel encapsulation reduces lead leakage by three orders of magnitude. This work provides a strategy to simultaneously address lead leakage and stability for perovskite modules



Dally

# Enhanced Hole Injection via Perovskite Band Alignment for High- Performance Blue light-emitting diode

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Metal halide perovskite materials have drawn tremendous attentions in light-emitting diodes (LEDs) area owing to the superior color purity, tunable emission spectrum, and high photoluminescence quantum yields (PLQY)[1,2]. Profiting from the excellent photoelectric properties, the performance of perovskite light-emitting diode (PeLED) develops rapidly in the recent years, and the external quantum efficiencies (EQE) have exceeding 20% for devices with emission spectrum ranging from near-infrared to green[3,4]. Nevertheless, the device performance in the blue region still lags behind counterparts, owing to their extremely unbalanced carrier injection and low PLQY.

Here, we first put forward a simple and effective alkali halide ion intercalation method (AIIM) to mainly modulate the energy level of perovskite and modify the HTL properly, thus jointly reducing the energy barrier and facilitating hole injection. We show that the band alignment can be effectively tuned through precisely controlling the content of alkali halide. Benefiting from the favorable band alignment and almost barrier-free hole injection, the peak EQE values of blue PeLEDs with 473 nm, 464 nm, and 458 nm wavelengths are 6.32 %, 3.82 %, and 1.40 %, respectively, are achieved without passivation optimization. Our work provides a novel way to resolve the imbalance in carrier transport by modulating perovskite energy level without sacrificing optical performance and shed light on perovskite band alignment engineering toward efficient blue PeLEDs.

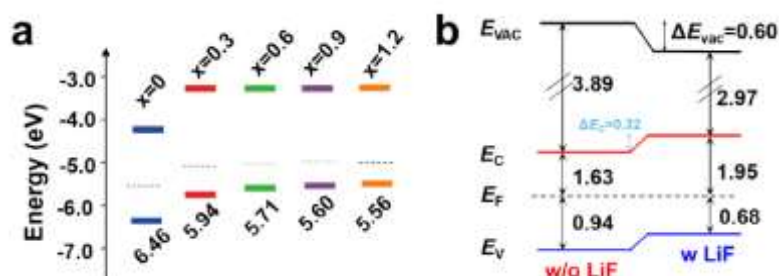


Figure 1 Energy level diagram of the perovskite with LiF intercalation.

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[3]Y. Cao, N. Wang, Q. Peng, J. Wang and W. Huang, *Nature* ( 2018), **562**, 249-253. [4] D. Ma, K. Lin, Y. Dong, Z. H. Lu, Z. Wei and E. H. Sargent, *Nature*, 2021, **599**, 594-598.

# Thermal Stability of Perovskite Solar Cells with Ionic liquid dopant to Spiro-OMeTAD

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Perovskite solar cells (PSCs) are attracting attention as next-generation solar cells because of their cost effective and high-power conversion efficiencies (PCEs). In the case of out-door use, PSCs are required the evaluation for environmental stability such as heat and light. In the regards, thermal stability issues of PSCs are well known, then one of these issues was caused from the components such as carrier transport layer in PSCs. In conventional PSCs, doping materials of hole transport layer (HTL) can be caused of the issue of thermal stability. To improve the initial PCE of PSCs, LiTFSI is used as a dopant to improve the conductivity of spiro-OMeTAD. However, LiTFSI is known to become  $\text{Li}^+$  and diffuse inside the perovskite layer and these phenomena decrease the PCE of PSCs. To improve the thermal stability of PSCs, it is necessary to avoid diffusion into the device by fixation  $\text{Li}^+$  at HTL [1]. In this study, we focused on the doping method of HTL in conventional PSCs for improving thermal stability. For fixation of the dopant in the HTL, bulky organic cations were investigated as the new dopants for PSCs. Since TFSI is an effective dopant for Spiro-OMeTAD, a combination of TFSI and organic cations were investigated to find the best dopants for spiro-OMeTAD. Our PSC structure is  $\text{FTO}/\text{SnO}_2/\text{Cs}_{0.05}\text{K}_{0.05}\text{FA}_{0.9}\text{PbI}_3/\text{spiro-OMeTAD}/\text{Au}$ . 1- Butyl-1-methylpyrrolidinium TFSI (Bmp-TFSI) and LiTFSI were used as dopants for HTL and compared, respectively. Optimized PSCs have PCE of 19.0% with LiTFSI and 17.9% with Bmp-TFSI. The solar cell performance with Bmp-TFSI was found to be equivalent to LiTFSI, and it was found that Bmp-TFSI can be a dopant. We also evaluated thermal stability of PSCs at 85°C and 30% RH. The PSC with Bmp-TFSI exhibited 70% of its initial properties after 500 hours at thermal stability test. On the other hand, the PSC with LiTFSI reduced to 30% of its initial performance just after 500 hours. These results suggest that the thermal stability of PSCs can be improved by using bulky organic ions as the dopant in HTL rather than small and diffusive ions such as Li.

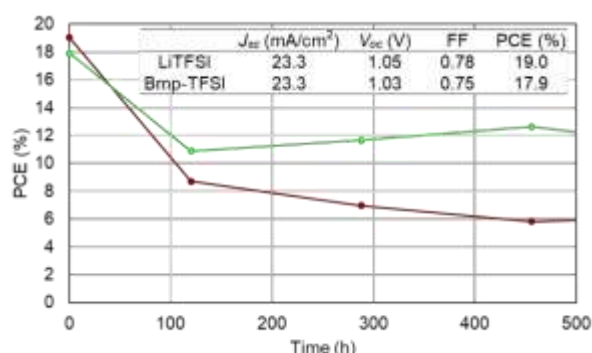


Figure 1 Thermal stability test of PSCs depending on HTL dopant.



# Perovskite orientation growth and bandgap optimization via thermal evaporation

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Vacuum evaporation has several advantages, such as potential for large-scale production avoid usage of solvents and compatibility with textured substrate enabling providing applications in monolithic perovskite (PVK)/Si tandem devices [1]. Therefore, it is important to study how to obtain thermally evaporated PVK with high film quality and suitable bandgap. As claimed in solution-based deposition methods, non-radiative recombination can be suppressed by means of crystal preferential growth [2]. However, manipulating PVK crystal orientation via thermal evaporation has hardly been addressed. Similarly, light induced instability of thermally evaporated wide-bandgap PVKs is also a challenge for tandem device applications [3]. We investigate both crystal growth orientation and light stability of thermally evaporated PVK layers.

Here, we manipulated the crystal orientation of thermally evaporated  $\text{Cs}_{0.15}\text{FA}_{0.85}\text{PbI}_{2.85}\text{Br}_{0.15}$  PVK layers from (110) to (100) and investigate its effect on their opto-electronic properties. The process starts by sequentially depositing lead iodide, formamidinium iodide, and cesium bromide with appropriate thicknesses to form ca 250-nm thick PVK layers. This process is repeated a second time to increase the total film thickness to 400-450 nm. Intermediate annealing treatments between the two depositions is found to control the orientation growth of the entire PVK layer as proven by 2DXRD measurements. Interestingly, (110)- and (100)-oriented PVK layers show comparable free carrier mobility of 30-35  $\text{cm}^2/(\text{Vs})$ , lifetimes (600-700 ns) according to photo-conductance measurements. Combined with the surface potential measurement, we conclude that the orientation growth of thermally evaporated PVKs mainly show difference in terms of surface properties, which dominates the optoelectrical property improvement in device level.

Using the same thermal evaporation approach, we also fabricated PVK layers with variable bandgaps ranging from 1.58 eV to 1.75 eV confirmed by the clear peak position shift in XRD and offset shift in UV-vis spectra. Photoluminescence measurements of varying band-gap perovskites PVK layers showed significant light induced activation accompanied with phase segregation which will be investigated in the next steps.

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# A Templating Approach to Controlling the Growth of Co-evaporated Halide Perovskites

SiYu Yan

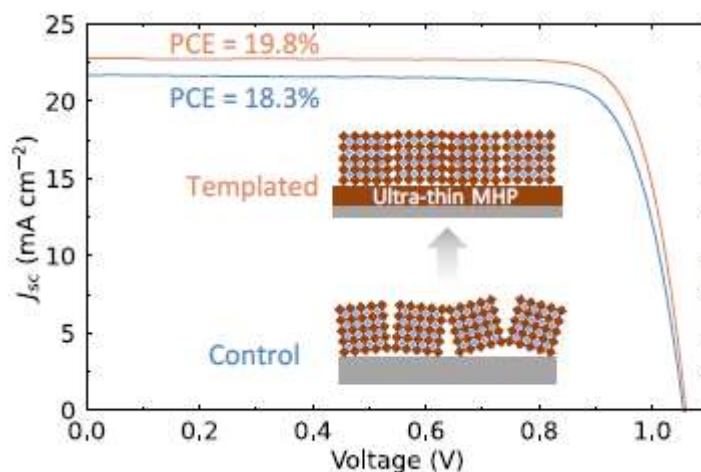
Jay B. Patel<sup>1</sup>, Jae Eun Lee<sup>1</sup>, Karim A. Elmostekawy<sup>1</sup>, Sinclair R. Ratnasingham<sup>2</sup>, Qimu Yuan<sup>1</sup>,  
Laura M. Herz<sup>1,2</sup>, Nakita K. Noel<sup>\*1</sup> and Michael B. Johnston<sup>\*1</sup>

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Metal halide perovskite semiconductors have shown significant potential for use in photovoltaic (PV) devices. While fabrication of perovskite thin-films can be achieved through a variety of different techniques, thermal vapour deposition is particularly promising, allowing for high-throughput fabrication and large-scale production [1]. However, the ability to control the nucleation and growth of these materials, particularly at the charge-transport layer/perovskite interface, is critical to unlocking the full potential of vapour-deposited perovskite PV [2].

In this study, we explore the use of a templating layer to control the growth of co-evaporated perovskite films, and find that such templating reproducibly leads to highly oriented films with identical morphology, crystal structure, and optoelectronic properties, independent of the specific substrate on which the perovskite was deposited. When incorporated into solar cells, devices based on this approach showed reproducible improvements, yielding vapour-deposited FA<sub>0.9</sub>CS<sub>0.1</sub>PbI<sub>3-x</sub>Cl<sub>x</sub> solar cells with steady-state solar-to-electrical power conversion efficiencies over 19.8%. Our findings provide a straightforward and reproducible method of controlling the charge-transport layer/perovskite interface in vapour-deposited perovskite solar cells, further clearing the path toward large-scale fabrication of efficient perovskite optoelectronic devices.



**Figure 1 Schematic diagram for controlling the growth of co-evaporated halide perovskites and improving the device performance by the templating approach**

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# Manipulation of the optoelectronic properties of layered hybrid perovskites by molecular intercalation

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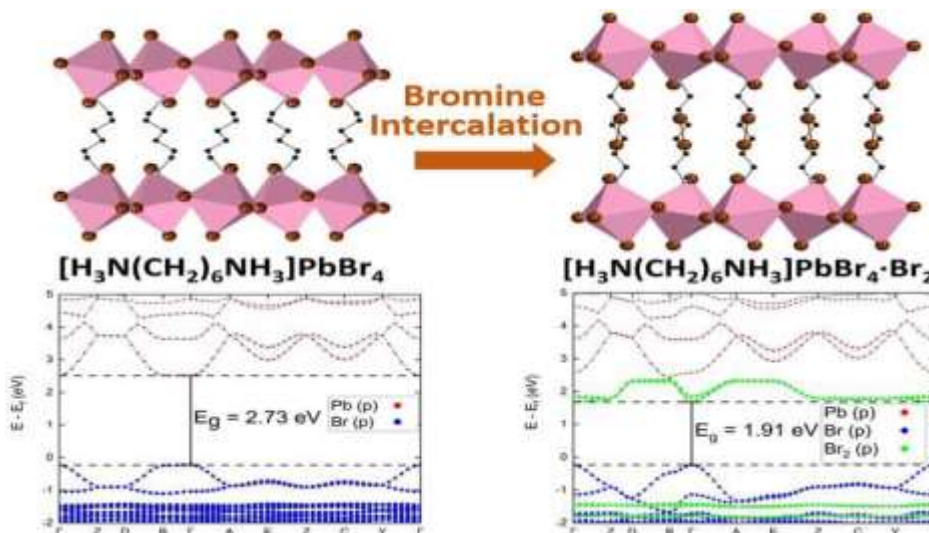
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Layered hybrid perovskites have received considerable attention due to the high tunability of their crystal structures, which in turn influences their physical properties. However, layered hybrid perovskites with single inorganic sheets (denoted as  $n = 1$ ) are hardly considered as light absorbers in solar cells, despite having good stability in air or humid atmospheres, due to their large bandgap ( $E_g$ ) and high exciton binding energy ( $E_b$ ).

Here, an alternative method is used to decrease the  $E_g$  of traditional  $n = 1$  perovskites: using halogen molecule intercalation [1]. For example, a bromine molecule could be inserted between the inorganic layers of hybrid perovskite  $[\text{H}_3\text{N}(\text{CH}_2)_6\text{NH}_3]\text{PbBr}_4$  and was stabilised by the formation of halogen bonds with  $\text{PbBr}_6$  containing inorganic layer. Crystallographic and computational studies were used to show that a new conduction band was provided by the guest bromine molecules during the intercalation. Also, a significant decrease in effective mass was observed. Therefore, compared with  $[\text{H}_3\text{N}(\text{CH}_2)_6\text{NH}_3]\text{PbBr}_4$ , the resulting crystalline material,  $[\text{H}_3\text{N}(\text{CH}_2)_6\text{NH}_3]\text{PbBr}_4 \cdot \text{Br}_2$ , has greatly lower bandgap and resistivity, but a higher mobility/ charge carrier concentration. Additionally,  $[\text{H}_3\text{N}(\text{CH}_2)_6\text{NH}_3]\text{PbBr}_4 \cdot \text{Br}_2$  has considerable stability in humid atmospheres, which proved that intercalation could be a potential method to design new photovoltaic materials.



[1] Lin-Jie Yang, Wenye Xuan, et al, *Chemistry of Materials* (2023), in press.

# Laminated Perovskite Solar Cells with Enhanced Stability and Performance via Thermocompression Bonding

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Perovskite solar cells (PSCs) are showing high efficiency of 26% for single-junction solar cells and 33.7% for tandem devices with silicon solar cells in small-area thanks to advances in materials and processes. In order to commercialize solar cells, the long-term stability against heat, moisture, and oxygen should be ensured. Further improvement of materials and device technology including encapsulation that protects devices from degradation factors are required, and these technologies should be simple, reproducible, and cost-effective. In this study, we present the simple but novel methods to protect materials and perovskite solar cells devices from degradation; Self-sealing device formation technology through thermocompressing lamination process will be demonstrated.

To enhance the performance of PSCs, the interfacial defects should be passivated. Additional coating or additive engineering for the perovskite films have been generally employed to passivate the defects. Here we identify that defect density in bulk and on interfaces of the perovskite are also effectively reduced by thermocompression. We extensively investigate the adjustment of chemical and physical properties in the perovskite layer by thermocompression bonding: larger grain size and lower trap density in its bulk; and higher adhesion, more hydrophobic, and suppressed ion migration at the interface with charge transport layers. In addition, self-sealing devices through thermocompressing between perovskite layers on glass substrates is demonstrated. The semitransparent PSCs with a wide-bandgap perovskite ( $E_g \sim 1.67$  eV) shows a power conversion efficiency of 17.24% and maintains the long-term stability with PCE > ~90% in the 85 °C shelf test for over 3000 hours and with PCE > ~95% in the MPPT test under AM 1.5 G, 1-SUN illumination for over 600 hours.

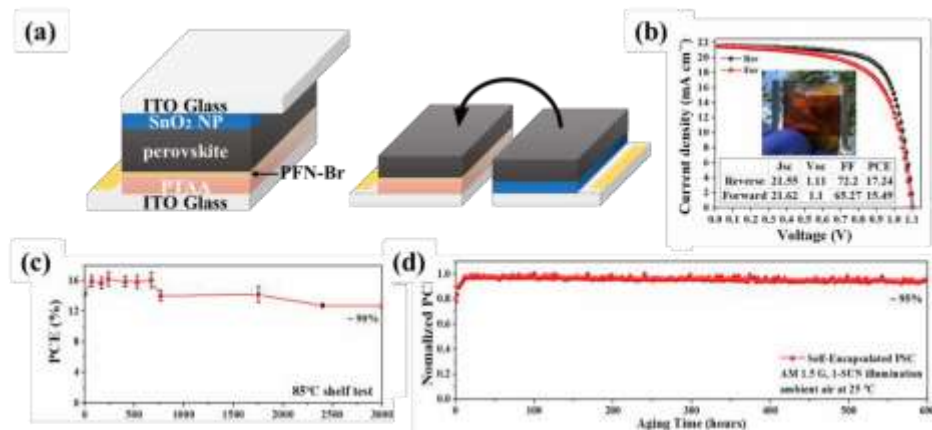


Figure 1. Perovskite solar cells fabricated by thermocompression bonding

# Impact of charge transport at the interfaces of lead halide perovskite solar cells

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During the past decade, lead halide perovskite has gained attention as a promising light absorbing material for photovoltaic applications due to its optoelectronic characteristics. Rapid advances in the perovskite material and device have enhanced power conversion efficiency from 3.8 to 26.0 % as well as improved device stability. Throughout the various perovskite solar cell (PSC) device architectures, the n-i-p device is regarded as the normal structure which consists of a transparent conductive oxide (TCO), electron transport layer (ETL), light absorbing perovskite layer, hole transport layer (HTL), and back contact electrode. Here charge transport at the interfaces must be considered as separating and extracting and transferring photogenerated carriers can be minimized by interfacial charge accumulation and recombination. Nevertheless, an understanding of charge transport between the interfaces is still lacking. We have reported that a space charge layer is formed between ITO and SnO<sub>2</sub>, leading to electron depletion and directly affecting device performance [1]. The space charge effect between SnO<sub>2</sub> and methylammonium lead iodide (MAPI) has also been explored. We investigated the surface property of SnO<sub>2</sub> and its interface effect with MAPI by first exploring the adsorption behavior of SnO<sub>2</sub> nanoparticles with FTIR and XPS measurements. Next, to identify charge distribution at the interface between SnO<sub>2</sub> and MAPI, TEM, XPS, AFM, and electrical measurements of the thickness dependent MAPI/SnO<sub>2</sub> samples were performed. Our work will provide a deeper understanding of the space charge effect at interfaces of lead halide perovskites-based devices and the material itself.

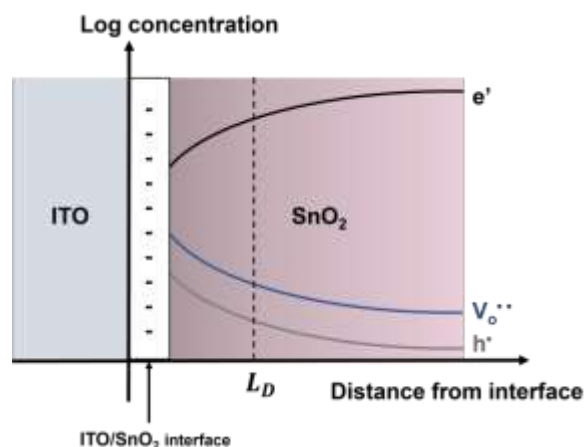


Figure 1 Schematic image of the SCL and expected carrier distribution at the ITO/SnO<sub>2</sub> interface.

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# Thermally Stable All-vacuum-deposited Perovskite Solar Cells with Copper Phthalocyanine Hole Transport Layer

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Vacuum deposition is a solvent-free method well-suited for the uniform growth of metal-halide perovskites (MHPs) thin films [1] and charge-transport layers. Vacuum-based methods offer a diverse array of advantages, including precise control of layer thickness, excellent homogeneity of the formed thin film, and the flexibility to grow multi-layer structures and larger-scale modules without the need to rely on complex choices of “orthogonal solvents”. However, most reports of high-efficiency solar cells based on vacuum-deposited MHP films often employ solution-processed hole transport layers (HTLs) such as PTAA or Spiro-OMeTAD [2,3]. Not only are these HTLs relatively expensive, and the additional solution-processing step complicates the overall fabrication process, but also more critically, materials such as Spiro-OMeTAD are prone to degradation under different environmental stressors of temperature and humidity, and thus curtailing the operational lifetime of these devices. We investigated organometallic copper phthalocyanine (CuPc) and zinc phthalocyanine (ZnPc), deposited via the thermal-evaporation method, as alternative, low cost, and durable HTLs in all-vacuum-processed solvent-free  $[\text{CH}(\text{NH}_2)_2]_{0.83}\text{Cs}_{0.17}\text{PbI}_3$  (FACsPbI<sub>3</sub>) perovskite solar cells. We reveal that the CuPc HTL demonstrated improved compatibility and performance in an ‘inverted’ p-i-n photovoltaic device, in comparison with ZnPc. Furthermore, we thoroughly examined the long-term stability of these all-vacuum-deposited devices under a range of testing conditions. Importantly, unencapsulated devices as large as 1 cm<sup>2</sup> exhibited outstanding thermal durability, demonstrating no observable degradation in efficiency after more than 5000 hours in storage and 3700 hours under 85 °C heat-stressing in N<sub>2</sub> atmosphere [4]. In addition, we uncover the striking differences in the sticking, adhesion, and nucleation dynamics of the organic perovskite precursor, formamidinium iodide (FAI), to various HTLs. We highlight the impact of varying sticking characteristics to the stoichiometry of the co-evaporated perovskite thin films. We believe that this finding epitomises the importance of optimising growth parameters specific to individual charge transport layer if FAI is to be used as a precursor in any co-evaporated perovskite [4].

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# Enhanced Hole Mobility of p-Type Materials by Molecular Engineering for Efficient Perovskite Solar Cells

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Star-shaped triazatruxene derivative hole-transporting materials (HTMs), TAT-TY1 and TAT-TY2, containing electron-rich triazatruxene cores (5,10,15-trihexyl-10,15-dihydro-5H-diindolo[3,2-a:3',2'-c]carbazole, TAT-H) and donor carbazole moieties were synthesized and successfully used in triple-cation perovskite solar cells [1]. All the HTMs, including the TAT-H main core had suitable highest occupied molecular orbitals (HOMOs) for perovskite (TAT-H:  $-5.15$  eV, TAT-TY1:  $-5.17$  eV, and TAT-TY2:  $-5.2$  eV). Steady-state and time-resolved photoluminescence results revealed that hole transport from the valence band of the perovskite into the HOMO of the new triazatruxene derivatives was more efficient than that of TAT-H. Furthermore, n-hexylcarbazole and 9-phenylcarbazole substitution to TAT-H was altered the crystalline nature of TAT-H main core that resulted a smooth and pinhole-free thin film morphology. As a result, TAT-TY1 and TAT-TY2 had power conversion efficiencies of up to 17.5% and 16.3%, respectively, compared to the reference Spiro-OMeTAD. These results demonstrate that the new star-shaped triazatruxene derivative HTMs can be synthesized without using complicated synthesis strategies.

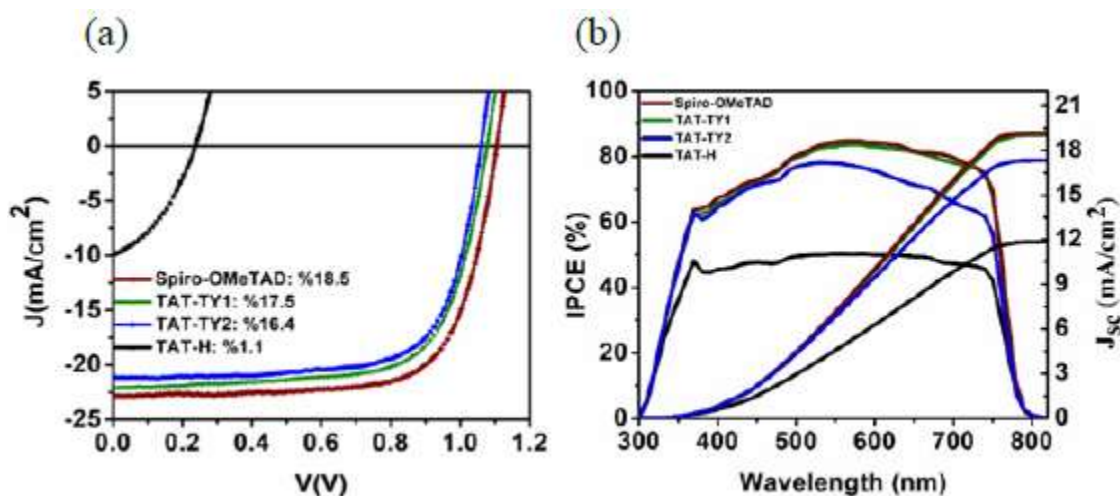


Figure 1 (a) Reverse bias J–V characteristics of PSCs containing the doped HTMs (b) the corresponding integrated  $J_{sc}$  values obtained from the IPCE measurements.

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# Study of co-evaporated $\alpha$ -FAPbI<sub>3</sub> perovskite growth as function of time and temperature deposition

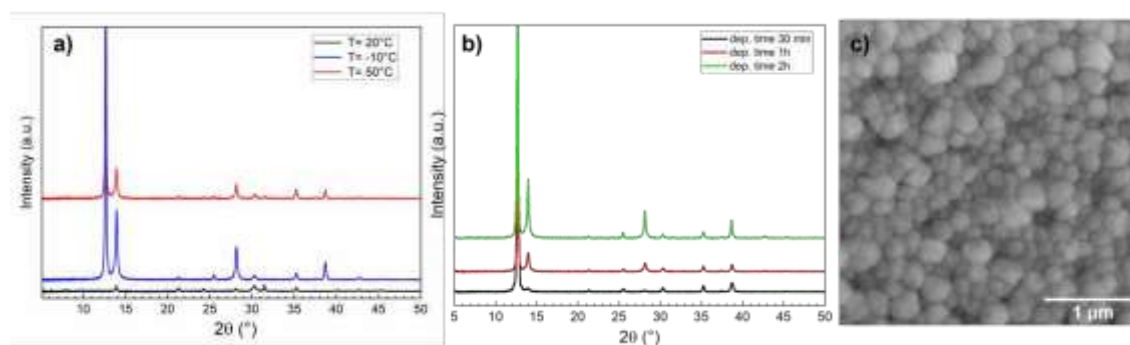
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To date, the fabrication of organic-inorganic perovskite solar cells (PSCs) has been mostly based on solution process although it presents severe drawbacks for industrial large area production. Co-evaporation represents a solvent-free and high-throughput technique for fabricating highly uniform, pin-hole free and smooth thin perovskite films [1]. The major difficulty in co-evaporation resides in the control of the organic component in respect to the inorganic one together with an accurate knowledge of the interfaces structure [1]. The deposition mechanism by double sources co-evaporation of organic formamidinium iodide (FAI) and inorganic lead iodide (PbI<sub>2</sub>) to deposit perovskite FAPbI<sub>3</sub> (FAPbI<sub>3</sub>) films is investigated as function of substrate temperature and deposition time. In fig.1 diffraction patterns of FAPbI<sub>3</sub> films evaporated on poly[bis(4-phenyl)(2,4,6-trimethylphenyl) amine (PTAA) deposited by spin-coating on glass/ITO are reported. After the post annealing at 150 °C for 15 minutes, peaks related to the  $\alpha$ -phase of FAPbI<sub>3</sub> perovskite are present together with intense PbI<sub>2</sub> peaks. The presence of an unconverted PbI<sub>2</sub> phase could be either a result of evaporation process or of post annealing due to the volatile formamidinium property [2]. Varying the substrate temperature, the incorporation of FAI is thermally activated and the intensity ratio between PbI<sub>2</sub> peak and (001) FAPbI<sub>3</sub>  $\alpha$ -phase peak is slightly increased pointing towards an enhancement of the cubic perovskite growth [3].



**Figure 1** a) X-ray diffraction patterns of FAPbI<sub>3</sub> perovskites deposited at different substrate temperatures; b) X-ray diffraction patterns of FAPbI<sub>3</sub> perovskites deposited at 60 °C for different deposition times; c) Scanning electron microscope image of the surface morphology of a thin film of FAPbI<sub>3</sub> perovskite grown at a substrate temperature of 20°C.

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# Manipulation of Crystal Orientation and Phase Distribution of 2D Perovskite through Synergistic Effect of Additive Doping and Spacer Engineering

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2D perovskite formed by adding large organic spacer cations has become more popular in recent years. Although organic spacers can increase the stability against moisture, oxygen, heat and ion migration, the efficiency of 2D perovskite is still lagging behind that of its 3D perovskite counterpart. The reason is that the quantum and dielectric confinement inside the natural multiple quantum well structures of 2D perovskites hinders charge carrier transport. Therefore, knowing how to fabricate high quality films of quasi-2D perovskites with a vertical crystal orientation and gradient phase distribution is of vital importance, in order to balance the high stability and efficiency. In our work, PDMA (1,4-phenylenedimethan ammonium) was used as the large organic spacer to prepare Dion-Jacobson type quasi-2D perovskite (PDMA)(MA)<sub>n-1</sub>Pb<sub>n</sub>I<sub>3n+1</sub>. The bifunctional spacer forms strong hydrogen bonds without weak Van der Waals gaps and shorter interlayer distances compared to the Ruddlesden-Popper type monovalent spacer. The  $n=5$  film in reality comprises multiple phases with locally different  $n$  values, forming a gradient in the film thickness direction, with more high- $n$  or quasi-3D phase on top and more low- $n$  2D phase at the bottom. However, the crystal orientation is not all vertically aligned, and hinders the charge transport in vertical direction. We assumed that this random orientation originates from the missing bridging of the adjacent [PbI<sub>6</sub>]<sup>4-</sup> octahedrons by the PDMA spacer. Due to its low number of degrees of freedom, it cannot rearrange itself during the crystallization, losing the supramolecular organization and spatial regularity, while monovalent spacers with VdWs gaps are more tolerant to defects. By mixing the Dion-Jacobson type spacer PDMA and the smaller Ruddlesden-Popper type spacer PA (propylammonium), the combination led to well-defined crystallinity owing to well-matched interlayer distancing, and the crystal orientation was regulated in both the vertical and the horizontal directions. Combining this spacer engineering approach with the addition of MAI, the crystal orientation became vertically aligned. Moreover, the phases at the bottom side changed from low- $n$  ( $n=1, 2, 3$ ) to high- $n$  ( $n=4, 5$ ), potentially facilitating hole extraction between the interface with a hole transport layer, due to the more finely tuned band alignment.

Our work aims at tuning the crystal orientation and phase distribution of quasi-2D perovskites from random, to regulated and preferential. Through synergistic strategies based on both internal precursor engineering and external processing methods, our work sheds light on the crystallization behaviour of quasi-2D perovskite, and further paves the way for highly stable and efficient perovskite devices.

## Ultrathin semitransparent perovskite solar cells

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Metal halide perovskites are of great interest for application in semitransparent solar cells due to their tunable bandgap and high performance. However, fabricating high-efficiency perovskite semitransparent devices with high average visible transmittance (AVT) is challenging because of their high absorption coefficient. One of the most promising approaches to increase the AVT of the devices is to decrease the perovskite active layer thickness. The realization of this approach is, however, complicated by the difficulty of depositing ultrathin compact perovskite films (<50 nm) by either solution processing or thermal evaporation. Here, we demonstrate the importance of controlling the perovskite growth mode in order to deposit continuous, smooth and homogeneous ultrathin perovskite films. Specifically, we show that the additive-assisted columnar growth of CsPbI<sub>3</sub> perovskite by thermal evaporation enables the formation of compact 10 nm thin films with excellent optoelectronic quality. When integrated into a p-i-n device structure with an optimized transparent electrode, these ultrathin layers result in an impressive open-circuit voltage (VOC) of 1.08 V and a fill factor (FF) of 80%. Consequently, a power conversion efficiency of 3.6% with an AVT of 54% is demonstrated, paving the way for their potential utilization in smart windows, light-emitting diodes, and tandem device applications.

# A robotic platform assisted perovskite materials synthesis

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Robotic platform for replace the trial-and-error synthesis and labor-intensive characterization underpin many aspects of laboratory automation, from hypotheses generation by data mining, experimental design by robotic system, and results interpretation by machine learning [1]. Due to the inherent multi-parameterized complexity of perovskite materials, it necessitates the upgradation of highly intelligent, robust, yet capability-multifarious robotic platform. To achieve digital manufacturing of perovskite materials, we develop a robotic platform through a framework consisting of data-driven automated synthesis, robot-assisted controllable synthesis, and machine learning models facilitated inverse design. We demonstrate this platform by synthesizing perovskite materials to show a new data-driven robotic synthesis approach. Firstly, an initial choice of key synthesis parameters was acquired through data mining of the literature. Secondly, automated synthesis and in situ characterization with further ex situ validation was then carried out and controllable synthesis of perovskite materials with the desired morphologies/properties was accomplished. Finally, to achieve morphologies/properties-oriented inverse design, correlations between the morphologies/properties and structure-directing agents are identified by machine-learning models trained on a continuously expanded experimental database. Thus, the developed robotic platform with a data mining–synthesis–inverse design framework is promising in data-driven digital manufacturing of perovskite materials.

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# Many-body Correlations and Exciton Complexes in CsPbBr<sub>3</sub> Quantum Dots

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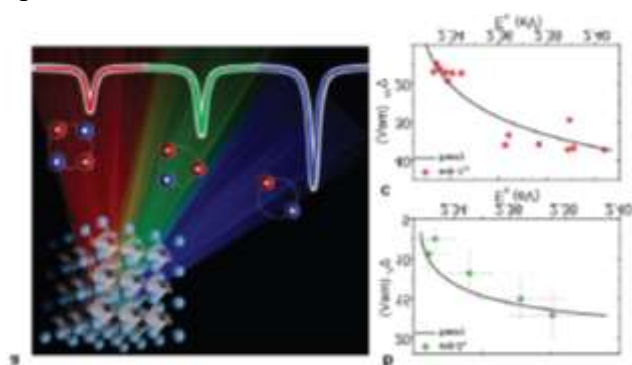
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All-inorganic lead-halide perovskite (CsPbX<sub>3</sub>, X = Cl, Br, I) quantum dots (QDs) have emerged as a competitive platform for various optoelectronic applications e.g., LEDs featuring narrow emission[1] and quantum light sources[2-3]. Many-body interactions and quantum correlations among photogenerated exciton complexes (see Figure 1a) play an essential role, e.g., by determining the laser threshold, the overall brightness of LEDs, and the single-photon purity[2,4] in quantum light sources. In this work[5], by combining single-QD optical spectroscopy performed at cryogenic temperatures in combination with configuration interaction (CI) calculations, we address the trion and biexciton binding energies and unveil their peculiar size dependence. We find that trion binding energies increase from 7 meV to 17 meV for QD sizes decreasing from 30 nm to 9 nm (see Figure 1b), while the biexciton binding energies increase from 15 meV to 30 meV (see Figure 1c), respectively. CI calculations quantitatively corroborate the experimental results and suggest that the effective dielectric constant for biexcitons slightly deviates from the one of the single excitons, potentially as a result of coupling to the lattice in the multiexciton regime. Our findings provide a deep insight into the multiexciton properties in all-inorganic lead-halide perovskite QDs, essential for classical and quantum optoelectronic devices.



**Figure 1. a) Sketch of the many-body interactions among photogenerated exciton complexes. b) Size-dependent trion binding energies ( $\Delta\nu^*$ ) in CsPbBr<sub>3</sub> QDs. c) Size-dependent biexciton binding energies ( $\Delta\nu\nu$ ) in CsPbBr<sub>3</sub> QDs.**

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# Impact of Low-Temperature Seed-Assisted Growth on the Structural and Optoelectronic Properties of MAPbBr<sub>3</sub> Single Crystals

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Perovskite single crystals are excellent candidates for photodetector applications due to their superior optoelectronic properties, including lower trap densities and longer diffusion lengths. Numerous growth methods have been developed to synthesize perovskite single crystals, however, the crystalline growth process to obtain high-quality single crystals is hard to control [1]. In this work, we have introduced a low-temperature seed-assisted inverse temperature crystallization (ITC) method for the growth of MAPbBr<sub>3</sub> single crystals. We have thoroughly examined the actual impact of seed-assisted growth on the final optoelectronic characteristics of MAPbBr<sub>3</sub> single crystals, in contrast to the nucleation-assisted approach. Compared to the conventional nucleation-assisted ITC growth at higher temperatures, this method has yielded single crystals of superior quality, with a significantly lower lattice strain as determined by X-ray diffraction (XRD) and enhanced photoluminescence response. Temperature-dependent space charge limited current (TM-SCLC) analysis further confirms these results, showing trap densities of  $9.47 \times 10^9 \text{ cm}^{-3}$  for seeded crystal growth compared to  $3.2 \times 10^{10} \text{ cm}^{-3}$  for the nucleation-assisted growth, as well as a lower trap energy level for the seeded crystal [2]. Furthermore, as a proof of concept, both seeded and unseeded single crystals are incorporated into photodetector devices. Interestingly, the seeded single crystals have exhibited higher detectivity (D) and responsivity (R) values than the unseeded ones. These findings highlight the importance of low-temperature kinetics during seed-assisted ITC on the final properties and applications such as photodetectors.

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# Optical and electrical optimization of the electron-selective top contact for perovskite single-junction and perovskite/silicon tandem solar cells

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Today's high-efficiency monolithic perovskite/silicon tandem solar cells typically comprise an electron-selective top contact of the perovskite subcell consisting of a C<sub>60</sub> fullerene electron-transport and a tin oxide (SnO<sub>x</sub>) buffer layer. While the C<sub>60</sub> layer is important for the efficient extraction of electrons from the perovskite absorber the SnO<sub>x</sub> layer is ascribed to function as protection layer to avoid damage through the subsequent transparent conductive oxide (TCO) sputter process and as diffusion barrier that improves the long-term operational stability [1-3]. However, although this design has proven to be highly suitable for p-i-n perovskite single-junction and perovskite/silicon tandem solar cells both layers introduce current limiting optical losses. The atomic layer deposition (ALD) of SnO<sub>x</sub>, moreover, potentially limits the devices' electrical performance due to the degradation of the perovskite absorber through a reaction with tetraakis(dimethylamino)tin (TDMASn) precursor [4]. In this contribution, we investigate the effect of the C<sub>60</sub> and SnO<sub>x</sub> layer thickness on the performance of tandem-relevant p-i-n perovskite single-junction and perovskite/silicon tandem solar cells. We find that a reduction in the C<sub>60</sub> and SnO<sub>x</sub> thickness can improve the optical and electrical solar cell performance due to a decrease in parasitic absorption and reflection losses as well as reduced exposure duration to perovskite-damaging ALD conditions. Using comprehensive photoluminescence (PL) analyses, water and dimethylformamide (DMF) exposure tests and contact angle measurements we analyze the SnO<sub>x</sub> film coverage on C<sub>60</sub> and find that thicknesses below 15 nm lead to non-closed films. Based on these results and additional long-term aging experiments we show that by applying a soft indium zinc oxide (IZO) sputter process the SnO<sub>x</sub> layer does not need to form a closed film in order to achieve superior solar cell performance and decent stability behavior. We further report that a critical minimum C<sub>60</sub> thickness is required to avoid deterioration of the open-circuit voltage (V<sub>oc</sub>) and fill factor (FF) most likely caused by facilitated diffusion of the ALD precursor to the perovskite. The results made a significant contribution to achieving a certified efficiency for perovskite/silicon tandem solar cells of 32.5 %.

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